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Kink band predictions in fiber composites using periodic boundary conditions

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ABSTRACT

A finite element based scheme for modelling kink band formation in fiber composites was developed. The model is computationally efficient by requiring only a few number of fiber/matrix layers representing the microstructure of the composite material. Yet, in comparison to finite element models including many fiber/matrix layers, the model is accurate by specifying periodic boundary conditions along the sides of the representative volume elements. These periodic boundary conditions allow for a rotation of the kink band after its initiation as observed in full-scale finite element calculations and experiments. Three different computational schemes for determining the kink band rotation have been suggested and compared.

1. Introduction

A critical failure mode leading to loss of load carrying capacity in composite materials under compression parallel to the fibers or layers is the formation of kink bands. The development of efficient numerical methods for studying kink band initiation and propagation in fiber composites have been the objective in a number of previous works. Finite element studies based on individually discretized, planar fiber and matrix models were reported in [1] and [2]. The models were extended to 3D simulations in [3]. It was in these studies established that a large number of layers had to be included in such computational models to eliminate effects from the sides of the representative volume element, which are taken as free edges. A drawback of such methods is obviously the computational effort needed to discretize large volumes of fiber/matrix layers in realistic simulations of composite structures and to avoid effects of boundary conditions imposed in the simulations of infinite kink band development. The study in [4] of kink band formation in realistic composite structures emphasizes the complexity of the problem and the need for developing efficient numerical schemes for predicting onset of failure.

An approach for overcoming the computational challenges involved in individually discretized fiber-matrix models for realistic geometries is described in [5]. Here, a coupling between a sub-model and a super element was introduced. Another approach is to introduce an effective constitutive model representing the composite material in the finite element formulation. Such a constitutive model for composite materials including non-local effects due to fiber bending stiffness was introduced in [6] and applied in finite element simulations of kink band formation in materials with variations in the local fiber orientation to simulate realistic composite structures. Input parameters in the model formulated in [6] are effective overall constitutive models for the composite material. The model incorporates a characteristic length scale and, thus, is capable of predicting the kink band width.

In [7] and [8], a constitutive model for a composite material including the constitutive responses of the fibers and the matrix was introduced and applied to study kink band initiation in perfect as well as imperfect structures. Input parameters to this model are individual constitutive models for the fibers and the matrix, along with volume fractions and continuity and equilibrium conditions at interfaces. The constitutive model was in [9] used to study the post buckling response and kink band broadening observed in ductile composite materials [10] and [11]. The constitutive model in [7] was in [12] implemented as a user defined material model in a commercial finite element software package, and was used to replicate the simple model predictions in [7] and [8]. The results based on this formulation were compared to the layer-wise individually discretized finite element calculations of [1] and [2] and were also used to study more realistic composite structures [13] where such approaches are computationally more efficient than individually discretized fiber-matrix layer models.

Recently, a mixture of the two approaches in [6] and [7] was formulated in [14]. A micro-mechanically non-local constitutive model for the composite incorporating a length scale to account for fiber bending stiffness effects was formulated. An implementation of the model in a finite element scheme was also done in [14] and demonstrated the capabilities of such models to predict the onset and evolution of a kink band. The results were in good agreement with individually discretized fiber-matrix layer models. Another recent contribution [15] introduces a length scale to model of kink band formation for damage growth by

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coupling strains to the width of the kink band.

Parallel to the efforts in developing constitutive models for fiber composites, some of which are mentioned above, other studies have focused on developing efficient computational tools for studying infinite kink band formation based on the individually discretized fiber-matrix layer formulation, see e.g. [16] and [17]. Here, a finite representative volume element for predicting the onset of kink bands was formulated as just a few layers of fibers and matrix but with periodic boundary conditions imposed to simulate the infinite kink band. The models imposing periodic boundary conditions at the sides of the representative volume elements are computationally more efficient than calculations performed assuming free boundaries since a large number of layers are required to eliminate the edge effects. However, the periodic boundary conditions, which should model a finite sample of an infinite specimen more appropriately, impose geometric restrictions on the kinematics associated with kink band formation. As an example, the previous models do not allow for a rotation of the kink band in the post-failure regime, i.e. the kink band orientation is fixed during the complete loading of the specimen. This is in contrast to observations on large-scale finite element simulations and experiments in e.g. [1] where the kink bands rotate in the post-failure regime. The consequence of fixing the kink band orientation is an unrealistic prediction of the load versus end shortening response for the composite.

In the present work, the focus is on developing a computational tool for infinite kink band analysis. It has the advantage of the model in e.g. [17] and [18] of being computationally efficient by just requiring a few fiber-matrix layers in a representative volume element with incremental periodic boundary conditions at the edges to model an infinite kink band. The model does not restrict the kinematics including the rotation of the kink band, and various strategies are pursued for letting the kink band orientation develop as deformation and failure in the composite progresses. The computational scheme is shown to be computationally efficient compared to previous models, and the predictions of load response is in good agreement with data from the literature.

2. Non-linear finite element analysis

An incremental finite element scheme for predicting the onset and development of a kink band in a fiber composite allowing for large deformations and large strains is based on the total Lagrangian formulation. The principle of virtual work is written in incremental form, which when using the summation convention for repeated index has the form

$$\int_{A_0}(S^{\alpha\beta}\tilde{\delta}\dot{E}_{\alpha\beta}+\dot{S}^{\alpha\beta}\tilde{\delta}E_{\alpha\beta})\mathrm{dA}_0=\int_{S_0}\dot{T}^{\alpha}\tilde{\delta}u_\alpha\mathrm{dS}_0-\left(\int_{A_0}S^{\alpha\beta}\tilde{\delta}E_{\alpha\beta}\mathrm{dA}_0-\int_{S_0}T^{\alpha}\tilde{\delta}u_\alpha\mathrm{dS}_0\right) \tag{1}$$

where A_0 is the undeformed area, $S^{\alpha\beta}$ are the contravariant components of the second Piola-Kirchhoff stress tensor, *PleaseCheck* denotes an incremental quantity, $\tilde{\delta}(\,)$ denotes a virtual quantity. Furthermore, in (1) T^α and u_α denote tractions pr. unit width and displacements, respectively, and S_0 denotes the undeformed circumference, and $E_{\alpha\beta}$ are the covariant components of the Green-Lagrange strain tensor, defined as

$$E_{\alpha\beta}=\frac{1}{2}(G_{\alpha\beta}-g_{\alpha\beta}) \tag{2}$$

Here $G_{\alpha\beta}$ and $g_{\alpha\beta}$ are the covariant components of the metric tensors of the deformed and undeformed configurations, respectively. The term in the parenthesis on the right hand side of (1) is included as an equilibrium correction term. At each increment in the loading procedure, equilibrium iterations are performed. The following relations between the strain tensors in (1) and the displacements are utilized in the finite element implementation using the notation $()_{,\alpha}$ for covariant differentiation with respect to coordinate $x\alpha$

$$\begin{aligned}E_{\alpha\beta}&=\tfrac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}+u^{\gamma}_{,\alpha}u_{\gamma,\beta})\\ \dot{E}_{\alpha\beta}&=\tfrac{1}{2}(\dot{u}_{\alpha,\beta}+\dot{u}_{\beta,\alpha}+\dot{u}^{\gamma}_{,\alpha}u_{\gamma,\beta}+u^{\gamma}_{,\alpha}\dot{u}_{\gamma,\beta})\\ \tilde{\delta}\dot{E}_{\alpha\beta}&=\tfrac{1}{2}(\dot{u}^{\gamma}_{,\alpha}\tilde{\delta}u_{\gamma,\beta}+\tilde{\delta}u^{\gamma}_{,\alpha}\dot{u}_{\gamma,\beta})\end{aligned} \tag{3}$$

The vector of displacement increments *PleaseCheck* are discretized using isoparametric 8-noded plane strain elements. The integrations in (1) needed to obtain the components of the stiffness matrix are carried out using reduced 2 × 2 Gauss integration. A forward Euler scheme is formulated for integration with respect to the pseudo-time variable *PleaseCheck* with equilibrium iterations at each increment. Increments are specified in an arc-length procedure introduced to handle snap-through and snap-back behavior in the load displacement response. An in-house finite element solver is developed for the purpose; all details of the implementation are explained in [18]. Thereby, full control of the boundary conditions imposed on the representative volume element is ensured which is important when introducing the rotating periodic boundary conditions later.

The constitutive response of both the fibers and the matrix is modelled by a finite strain version of J_2 deformation theory [19], which in 3D takes the following form for the tensor of instantaneous elastic-plastic moduli L^{ijkl} relating rates of Kirchhoff stresses, *PleaseCheck*, to rates of strains, *PleaseCheck*,

$$\begin{aligned}\dot{\tau}^{ij}&=L^{ijkl}\dot{E}_{kl}\\ L^{ijkl}&=\frac{E_s}{1+\nu_s}\left(\frac{1}{2}(G^{ik}G^{jl}+G^{il}G^{jk})+\frac{\nu_s}{1-2\nu_s}G^{ij}G^{kl}-\frac{3}{2}\frac{E_s/E_t-1}{E_s/E_t-(1-2\nu_s)/3}\frac{s^{ij}s^{kl}}{\sigma_e^2}\right)\\ &\quad-\frac{1}{2}(G^{ik}\tau^{jl}+G^{jk}\tau^{il}+G^{il}\tau^{jk}+G^{jl}\tau^{ik})\end{aligned} \tag{4}$$

Here,

$$\nu_s=\left(\nu-\frac{1}{2}\right)\frac{E_s}{E}+\frac{1}{2} \tag{5}$$

The secant modulus, E_s, and the tangent modulus, E_t, is evaluated from relating the effective stress, σ_e, where

$$\begin{aligned}(\sigma_e)^2&=\tfrac{3}{2}s_{ij}s^{ij}\\ s^{ij}&=\tau^{ij}-\tfrac{1}{3}G^{ij}\tau^k_k\end{aligned} \tag{6}$$

to a point on the uniaxial Cauchy stress, σ, vs. logarithmic strain, ε, curve which is approximated by a Ramberg-Osgood expression of the type

$$\varepsilon=\frac{\sigma}{E}+\frac{3}{7}\frac{\sigma_y}{E}\left(\frac{\sigma}{\sigma_y}\right)^n \tag{7}$$

Finally, the following relations between the Kirchhoff stress tensor, τ^{ij}, the Cauchy stress tensor, σ^{ij}, and the second Piola-Kirchhoff tensor, S^{ij}, are utilized

$$\tau^{ij}=\sqrt{\frac{\bar{G}}{g}}\sigma^{ij},S_{ij}=F^{-1}_{ik}\tau^{kl}F^{-1}_{jl} \tag{8}$$

where *PleaseCheck* and g are the determinants of the metric tensors ($G_{\alpha\beta}$ and $g_{\alpha\beta}$), and *PleaseCheck* are the covariant components of the inverse of the deformation gradient tensor. Two alternative plasticity theories have been compared to predictions based on (4). These are the finite strain versions of J_2 flow theory in [20] and the J_2 deformation theory [21]. Most previous work on kink band formation in polymer matrix composites have relied upon J_2 plasticity models and extensive experimental validation of the models for a PEEK matrix/carbon fiber system has been carried out in [1].

In the numerical procedure, the reference configuration for the undeformed geometry is a Cartesian frame so that $g_{\alpha\beta}$ in (2) has the components, $g_{11}=g_{22}=1$ and $g_{12}=g_{21}=0$. The incremental version of the virtual work principle (1) results in a linear set of equations for the nodal displacement rates in the FEM discretization of *PleaseCheck*.