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### Microstructure effects on transverse cracking in composite laminae by DEM

Yong Sheng<sup>a</sup>, Dongmin Yang<sup>a</sup>, Yuanqiang Tan<sup>b</sup>, Jianqiao Ye<sup>a,\*</sup>

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#### ABSTRACT

A particle discrete element method (DEM) was employed to simulate transverse cracking in laminated fiber reinforced composites. The microstructure of the laminates was modeled by a DEM model using different mechanical constitutive laws and materials parameters for different constituents, i.e. fiber, matrix and fiber/matrix interface. Rectangular, hexagonal and random fiber distributions were simulated to study the effect of fiber distribution on the transverse cracking. The initiation and dynamic propagation of transverse cracking and interfacial debonding were all captured by the DEM simulation, which showed similar patterns to those observed from experiments. The effect of fiber volume fraction was also studied for laminae with randomly distributed fibers. It was found that the distribution and volume fraction of fibers affected not only the transverse cracking path, but also the behavior of matrix plastic deformation and fiber/matrix interface yielding in the material.

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#### 1. Introduction

The inherent multi-phased microstructure of fiber reinforced composites, e.g., fiber volume fraction, fiber direction and interfacial strength, results in complex failure modes dominated by fracture of constituent elements. The damage evolution and failure mechanism of composites are obviously far more complex than those of monolithic materials due to the interactions of constituents. The complicated nature of failure/damage modes and physical composition of composite materials make the prediction and evaluation of progressive damage a challenging task. It is very important for material design and structural optimization in composite manufacturing to have the predictive capability on the dynamic failure/damage process. For instance, the properties of a laminate depend very much on the properties of its lamina and ply interface; the behavior of each lamina is, in turn, governed by its constituents, i.e. the properties of the fibers, the surrounding matrix, the interface and the relative amount of fibers and matrix in the lamina. When a composite is under external loading, damage, such as delamination, debonding, matrix cracking and fiber breakage, may occur. The accumulation of the damage during the loading process may eventually cause collapse of the whole material. Therefore a study of the damage or failure modes at micro scale with the consideration of microstructure is a more direct approach to predict the mechanical behavior of the composites.

Traditional micromechanical models focused mainly on the analysis of stress field [1–3], or predicting crack propagation using a prescribed failure criterion for composites with small numbers of fibers [4-6]. The ability to cope with inhomogeneity or/and disorder is essential in order to predict the damage process of a composite from micro-cracking to catastrophic failure. Transverse cracking, which normally is formed by matrix cracking and fiber/matrix interfacial debonding, is a familiar phenomenon in a lamina or laminated composite when it is subjected to transverse tension. Finite element method (FEM) has been widely used in this analysis on the basis of imposing various failure criteria [7-9]. However, many of these criteria do not have a rigorous physical basis that can be related to the microstructure of composite materials. Furthermore, the stress field that is calculated to meet the failure criteria of a composite is normally obtained by assuming that the material is not damaged. Thus stress redistribution in the material arising from, e.g., strain softening induced by localized damage cannot be taken into account. Some of the FEM models may agree well with experimental results, but it is very difficult for them to explain how the damage starts and develops in a composite during the entire loading process. Therefore, it is very challenging for a conventional continuum mechanics based numerical model to predict the whole dynamical damage/failure process, from matrix cracking initiation to final laminae/laminates collapse.

A fiber reinforced composites can be imaged as discrete fibers being inserted into a continuous matrix and bonded together by the interfaces between them. The discrete fibers interact with each other through the matrix between them. The analysis of the composite can be carried out through the analysis of the interaction of

<sup>&</sup>lt;sup>a</sup> School of Civil Engineering, University of Leeds, LS2 9IT, UK

<sup>&</sup>lt;sup>b</sup> School of Mechanical Engineering, Xiangtan University, Hunan 411105, China

<sup>\*</sup> Corresponding author. E-mail address: j.ye@leeds.ac.uk (J. Ye).

the discrete fibers. Since a large number of fibers are used in a fiber reinforced composite material, the interaction of these fibers was conventionally studied by the Monte-Carlo method [10,11]. However, the Monte-Carlo method cannot take into account the matrix effect, and the numerical results can hardly interpret the experimental investigations. On the other hand, discrete element method (DEM) [12] combined the statistical analysis with the concept of physical bonds from Molecular Dynamics (MD), and offered an intrinsic advantage over other numerical methods in modeling microscopic and multiphased materials. DEM was proposed by Cundall in the context of rock mechanics [12] and has been implemented in many other fields, such as geomaterials [13], granular materials [14], concrete [15], ceramics [16,17], particle-fluid [18] and particle-gas two phase flow [19]. Kim et al. [20,21] used DEM to simulate the damage of asphalt concrete which is a typical example of two-phase composite materials. Yang et al. [22] used DEM to simulate the dynamic process of microbond test of single fiber reinforced composite with the consideration of matrix cracking as well as fiber/matrix interfacial debonding. Donze et al. [23,24] simulated the impacts of rigid spherical nose shaped missiles on concrete beams with reinforcements. The existing studies concluded that DEM could provide unique insight into damage evolution at both micro and macro scales in the process of the dynamic characterization of fracturing. Van Mier et al. [25,26] used a lattice beam model, which is equivalent to the DEM model using regular particle arrangements, to study the fracture behavior of concrete from micro-cracking initiation and macro-crack failure in both two and three dimensions. Wittel et al. [27,28] has applied a lattice spring model, which is a simple form of DEM, to simulate ply transverse cracking of cross-ply laminates, in which the nodes represent fibers and the springs with random breaking thresholds represent the disordered matrix. It has been confirmed by the existing studies that DEM is particularly suitable to simulate dynamic instability in crack propagation and the collective behavior of many interacting cracks. However, the spring models used for the matrix and interface by Wittel et al. [27,28] are too simple to represent the mechanical properties of real materials and interfaces. Matrix cracking cannot be correctly simulated by this model and, only regular distribution of fibers with a fixed volume fraction can be considered.

In the research presented in this paper, DEM was used to simulate transverse cracking in laminae, including onset and propagation of the matrix cracking and fiber/matrix interface debonding. Composite laminae with regular distributions of fibers were modeled first and the numerical results were compared with the existing experimental results to validate the developed DEM model. The model was then modified to include random distribution of fibers with different fiber volume fractions. Based on the numerical results from the DEM modeling, the effect of microstructure of the composite laminae on the onset and the propagation path of transverse cracking, and the resulting residual damage within the material can be assessed. The DEM model proposed in this paper can be used for the analysis of more complex composite systems, such as cross-ply laminates.

#### 2. Discrete element method (DEM)

The particle discrete element method used in this research assumes that the particle elements are rigid spheroids (3D) or discs (2D), and can overlap or detach from each other. The contact forces between any two particles are determined from the overlap and relative movements of the particle pair according to a specified force–displacement law. In 2D DEM, the motion of a particle over a time step  $\Delta t$  is governed by the Newton's second law as below [12,14]:

Translational motion 
$$F_i = m(\frac{\Delta vi}{\Delta t} - g_i)$$
 (1)

Rotational motion 
$$M_a = I \frac{\Delta \omega_3}{\Delta t}$$
 (2)

where i (= 1, 2) denotes, respectively, the x-and y-co-ordinate directions;  $F_i$  is the resultant force of the particle;  $v_i$  is the translational velocity; m is the mass of the particle  $g_i$  is the body force acceleration vector (e.g., gravity loading);  $M_3$  is the out of balance moment referred to the out-of-plane axis;  $w_3$  is the rotational velocity about the out-of-plane axis;  $w_3$  is the rotational velocity about the out-of-plane axis;  $w_3$  is the rotational inertia of the particle;  $w_3$  time and  $w_3$  is the increment. Damping, e.g., local damping or viscous damping, can be added in the DEM model to dissipate the kinetic energy together with particles' frictional sliding, such that a steady-state solution can be obtained more efficiently [29]. Eqs. (1) and (2) are solved by a finite difference scheme. Both the specified force–displacement law and Newton's second motion law are used in the calculation cycle of the discrete element method.

DEM allows particles to be bonded together at contacts and to separate when the bond strength or energy is exceeded. Therefore it can simulate the motion of individual particles and also the behavior of a bulk material which is formed by assembling many particles through bonds at contacts with different constitutive laws. In a DEM model of bulk material, elementary micro scale particles are assembled to form the bulk material with macroscopic continuum behavior determined only by the dynamic interaction of particles [29,30]. Unlike the traditional solution using the strain and stress relations, contact properties are the dominating parameters in a DEM solution, combined with size and shape of the particles. Subject to external loading, when the strength or the fracture energy of a bond between particles is exceeded, flow and disaggregation of the particle assembly occur and the bond starts breaking. Consequently, cracks form naturally at micro scale. Hence, damage modes and their interaction emanate as the process of debonding of particles. The way that DEM discretizes a material domain gives the most significant advantage over the traditional continuum methodologies, as dynamic material behavior of composites, crack tip singularities and crack formulation criteria can all be avoided due to the naturally discontinuous representation of composite materials via particle assemblies.

In a DEM model for composite materials, damage initiation and propagation will take place at the particle contacts under the applied load. There is no requirement for additional failure criteria and the damage of different constituents can be taken into account simultaneously. The damage interaction will also be addressed through the dynamic motion of particles and contacts. The simulation results of a DEM model are naturally discrete and collected at microscopic level. The statistical analysis of the DEM results can also reveal material and structural behavior at macro scale by studying the bonds that have been broken or has yielded.

#### 3. DEM simulation of laminae under transverse tension

#### 3.1. Constitutive models

A DEM model of a solid material is usually constructed by packing discrete particles into an assembly through rectangular, hexagonal or random arrangement. Random arrangement is the most general approach in which the disperse particles are compacted or expanded to reach a dense contacting network, as shown in Fig. 1. Since a lamina is an inhomogeneous material which includes three phases: fiber, matrix and fiber/matrix interface, individual DEM models for each of the three phases are developed and virtual material tests (e.g., tensile and compressive tests) are carried out on all the phases, respectively, before the construction of the whole lamina model. The fiber material is represented by a parallel bond

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