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Abstract A micromechanical model for composite materials is proposed in which the components are assumed to obey continuum laws, and where the interfaces between the components are modelled with nonlinear springs. A homogenization procedure is used to obtain a constitutive relation of a fictitious homogeneous material body, that best represents the real heterogeneous composite. The latter relation shows a strain-softening behaviour which gives rise to mesh-dependent finite element solutions. A nonlocal formulation of this macroscopic relation can solve these problems.

1 Introduction

In continuum mechanics, the material behaviour is expressed by the constitutive equations. These equations describe the relation between, for example the Cauchy stress field and the linear strain field. For simple material behaviour, this relation can be determined experimentally, but for e.g. composite materials, this is very difficult. The reason is that during the deformation of a composite, several micromechanical failure mechanisms (like fibre-matrix debonding, matrix cracking, and fibre breaking) occur at the same time, and that the macroscopic behaviour strongly depends upon these mechanisms. In order to investigate this influence, it is necessary to use a micromechanical description of these kind of materials.

It is however, impossible to calculate the response behaviour of a composite, based on such a detailed description, because of the excessive computing time needed. Therefore, it is necessary to determine the material behaviour of a fictitious homogeneous material, that best represents the real heterogeneous material. Due to the micromechanical failure mechanisms, this fictitious material will show a strain-softening behaviour, so that strain-localization is likely to occur. This gives rise to numerical problems, in particular to mesh-dependent finite element solutions. These problems can be solved by introducing a nonlocal or a gradient dependent formulation

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of the macroscopic constitutive equation [2].

In the next section, we shall propose a micromechanical model for composite materials. We shall focus on the modelling of the interface between components of a composite, such as the fibre-matrix interface. The results of some finite element calculations, based on this model, are presented as well. In Sec. 3, the method of homogenization is discussed and problems with strain-softening and strain-localization are pointed out. Finally, in Sec. 4 some conclusions are drawn.

2 Micromechanical Modelling of Composites

In this section, we shall present a micromechanical model of a composite. The composite is taken to be a set of components, connected by interface layers. The latter may represent fibre-matrix interfaces, or cracks. We shall assume that the components of the composite obey the normal continuum mechanical laws, so that for each component we have the balance laws, the constitutive relations, and the kinematic relations. In addition to these partial differential equations, the components are subject to certain boundary conditions. These boundary conditions can either be *external*, that is, externally applied on the boundary if it coincides with that of the composite, or *internal*, on the boundaries with the interface layers, due to the interaction between two components. For the latter, two models are proposed in [6]. In these models, it is assumed that for each component B_k $(k = 1, 2)$, there exists a part Γ_k of its surface, the *interaction surface*, where the particle interacts with the surface of the other particle.

In the first model, the *continuous model*, each material point $\mathbf{x}_1 \in \Gamma_1$ on the interaction surface of B_1 interacts with a continuous set $S_2(\mathbf{x}_1, t) \subset \Gamma_2$ of material points on the surface of B_2. Hence, each material point $\mathbf{x}_2 \in \Gamma_2$ interacts with the continuous set

$$S_1(\mathbf{x}_2, t) = \left\{ \mathbf{x}_1 \in \Gamma_1 \;\middle|\; \mathbf{x}_2 \in S_2(\mathbf{x}_1, t) \right\} \subset \Gamma_1, \tag{1}$$

of material points on the surface of B_1.

The forces acting between two points are assumed to be conservative with respect to the distance between them, that is, there exists a function $U\colon [0, \infty) \to \mathbb{R}$, the *interaction energy*, such that the force that acts on a point P, at a distance $\mathbf{r}$ of a point P_0, due to its interaction with that point, is given by

$$\mathbf{F}(\mathbf{r}) = -\operatorname{grad} U(r) = -F(r)\,\mathbf{e}. \tag{2}$$

Here, $r = \|\mathbf{r}\|$, $\mathbf{e}$ is the unit vector in the direction of $\mathbf{r}$, and grad is the gradient operator with respect to $\mathbf{r}$. The function $F(r) = U'(r)$ is the magnitude of the force. The forces may be due to the molecular bonds between the particles, or they may represent the response of fibrils, formed between them, in cases of crazing, for example. In the former case, if the interface represents the weak Van der Waals interaction between the particles, then the function $U(r)$ is usually taken to be a Lennard-Jones potential,

$$U(r) = U_0 \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^{6} \right], \tag{3}$$

where r_0 is the equilibrium distance of the bond, corresponding to minimal potential energy $-U_0$.

In the second model, the *discrete model*, the interaction surfaces Γ_k of the particles are subdivided into a finite number of disjoint subsets C_{kn}, $(n = 1, 2, \ldots, N_k)$, called *cells*, such that Γ_k is the union of these cells. Each cell C_{1n_1} on the surface of B_1 interacts with a family $\{ C_{2n_2} \mid n_2 \in I_{2n_1} \}$ of cells of B_2, where I_{2n_1} is some subset of $\{1, 2, \ldots, N_2\}$, and, hence, each cell C_{2n_2} interacts with the family $\{ C_{1n_1} \mid n_1 \in I_{1n_2} \}$, where I_{1n_2} is given by

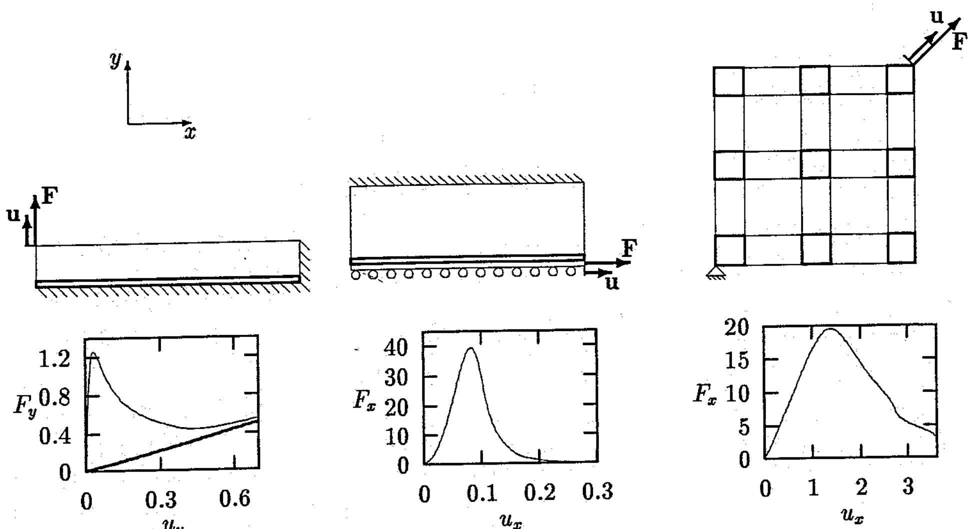
$$I_{1n_2} = \Big\{ n_1 \in \{1, 2, \ldots, N_1\} \Bigm| n_2 \in I_{2n_1} \Big\}. \tag{4}$$

For the interaction between two cells, we choose in each cell C_{kn} a fixed point $\boldsymbol{\xi}_{kn}$, the *interaction point* of the cell. If C_{kn} and C_{lm} are two interacting cells, with interaction points $\boldsymbol{\xi}_{kn}$ and $\boldsymbol{\xi}_{lm}$, respectively, we define the (constant) force distribution on C_{kn}, due to the interaction with C_{lm}, to be $\mathbf{F}(\boldsymbol{\xi}_{kn} - \boldsymbol{\xi}_{lm})|C_{lm}|$, where $|A| = \int_A d\sigma$ is the area of the surface A.

By calculating the total force in each point of the interaction surface, the internal boundary loads are obtained. As shown in [6], the interface layers are globally in equilibrium, that is, the sum of the total forces on Γ_1 and Γ_2 vanishes.

With these models, several interface elements have been formulated, including a four noded quadrilateral, two dimensional plane element, in case the particles are in a plain strain or plane stress state, and a two-and-a-half dimensional one, that can be used in two dimensional calculations on fibrous materials to model the interface between two overlapping fibers. To test these elements some calculations were carried out, in which the components were taken to be homogeneous isotropic elastic bodies. Only the discrete variants of the models were used. For the interaction energy between two points, the Lennard-Jones potential (3) was taken. In Fig. 1, the initial configurations of the models are depicted, and the relevant forces are plotted as functions of the prescribed displacements. The regions marked by the thick lines in the figures are the interface layers.

The first simulation (Fig. 1a) is that of a peel-off test. Here, an elastic beam is connected to a rigid surface with a layer of two-dimensional interface elements , while the vertical displacement of the upper left corner is prescribed. The right boundary of the beam is clamped. The second example (Fig. 1b) is a fibre pull-out test. In this test, a fibre, initially embedded in a matrix, is being pulled out. Symmetry conditions are taken into account. In the last calculation (Fig. 1c), a three by three square network of overlapping fibres is modelled under a diagonal loading. The thick drawn squares, where two fibres overlap, are the interaction surfaces of the fibres. We



(a) peel-off test (b) fibre pull-out test (c) fibre network

Figure 1 The results of finite element calculations with interface elements on (a) a peel-off test, (b) a pull-out test, and (c) a fibre network. The regions marked by the thick lines are the interface surfaces. The results of the calculations are depicted in the plots below the figures.

assume that at those points each (two-dimensional) fibre stays in a fixed plane, and that the two planes are parallel at a fixed distance of each other. The two quadrilateral elements that are used to model the fibres in the squares are then connected by a two-and-a-half dimensional interface element. The lower left corner of the network is fixed, while the displacements of the upper right corner are prescribed along the diagonal.

In all three examples, we see that the forces initially increases, but that at a certain displacement, the loads starts to decrease (strain softening). From the peel-off test we can see that this is caused by the interface. In the plot of Fig. 1a, the thick line shows the vertical component of the force as a function of the vertical displacement of the upper left corner of the beam, in case the interface layer between the beam and the surface is omitted.

3 Homogenization and Strain Softening

As we already have pointed out in the introduction, due to the excessive computing time needed, it is almost impossible to calculate the material behaviour of a composite, based on a detailed description of the microstructure. Therefore, we need to determine the material properties of a fictitious homogeneous material, that best represents the

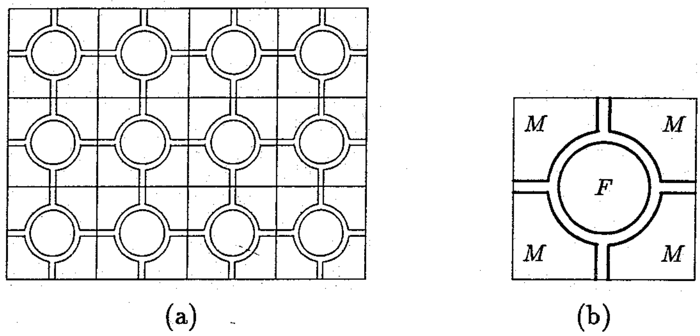


Figure 2 A statistically homogeneous fibre reinforced composite (a) and its representative volume element (b). The F and M denote fibre and matrix material, respectively, and the region marked by the thick lines are fibre-matrix and matrix-matrix interfaces. The latter is to simulate matrix cracking.

real heterogeneous structured material.

Following Maugin [4], we assume that the material is *statistically homogeneous*, so that a representative volume element (RVE) can be recognized (cf. Fig. 2). The macroscopic quantities are defined by the volume average over the RVE of the respective microscopic quantities. That is, if $\phi(\mathbf{x}, \mathbf{y})$ is a microscopic quantity (stress, strain, etc.), at a point $\mathbf{y}$ of the RVE, belonging to point $\mathbf{x}$ of the fictitious material body, then the macroscopic quantity $\bar{\phi}(\mathbf{x})$, at the point $\mathbf{x}$ is defined by

$$\bar{\phi}(\mathbf{x}) = \frac{1}{|\mathrm{RVE}|} \int_{\mathrm{RVE}} \phi(\mathbf{x}, \mathbf{y})\, d\mathbf{y}. \tag{5}$$

The RVE is modelled micro mechanically, and by applying the average strain $\bar{\varepsilon}(\mathbf{x})$ on the RVE (by means of the appropriate boundary conditions) the average stress $\bar{\sigma}(\mathbf{x})$ is computed. In this way a (formal) relation between $\bar{\varepsilon}(\mathbf{x})$ and $\bar{\sigma}(\mathbf{x})$ is obtained:

$$\bar{\sigma}(\mathbf{x}) = \mathbf{G}(\mathbf{x}, \bar{\varepsilon}(\mathbf{x})). \tag{6}$$

This relation is used as a constitutive equation for the fictitious material.

Several theories exist that yield analytic expressions for $\mathbf{G}$, in case the material behaviour of the RVE is linear elastic or perfectly plastic (cf. [3], [4]), or for plastic hardening materials with periodic structures (cf. [5]). However, as we see from the previous calculations (Fig. 1), the RVE shows a strain softening behaviour, in which case the material behaviour is neither elastic, nor plastic hardening, and because of the strain localization that will occur, the structure of the material, although maybe initially periodic, will not stay periodic. Hence, it will be very difficult to obtain an analytical expression for $\mathbf{G}$, in this case.

There are two possible (numerical) solutions for this problem. The first one is to use a so-called Multi-Level Finite Element Method (MLFEM). In this method, the formal constitutive relation (6) is used to formulated an element for the fictitious material. The stress in an integration point of that element is calculated by a second finite element analysis of a RVE, by imposing the strain in that integration point on the RVE, and by averaging the calculated stress field. However, the computing time needed for such calculations is still enormous, so this method is not very usable either.

A second approach is to determine an explicit expression for $\mathbf{G}$, by means of a parameter estimation method, on a (well) chosen expression. For example, the RVE depicted in Fig. 2 is isotropic, so if we assume that its behaviour is elastic, the general constitutive equation is given by

$$\bar{\boldsymbol{\sigma}}(\mathbf{x},t) = a_0\mathbf{I} + a_1\bar{\mathbf{B}}(\mathbf{x},t) + a_2\bar{\mathbf{B}}^2(\mathbf{x},t), \tag{7}$$

where $\bar{\mathbf{B}}(\mathbf{x},t)$ is the left Cauchy-Green tensor, which, for small strains is related to $\bar{\boldsymbol{\varepsilon}}(\mathbf{x},t)$ by $\bar{\mathbf{B}}(\mathbf{x},t) = \mathbf{I} + 2\bar{\boldsymbol{\varepsilon}}(\mathbf{x},t)$, and where a_0, a_1, and a_2 are functions of the invariants of $\bar{\mathbf{B}}(\mathbf{x},t)$. With a good choice for the functions a_i, the parameters therein can be determined from micromechanical calculations on the RVE.

Suppose now that we have found (analytically or numerically) a relation between the average stress and the average strain of an RVE. As illustrated by Fig. 1, this relation has a strain softening behaviour. Thus, due to e.g. non-uniform material properties, one material point (or line, or area) will be the weakest, that is, the maximum stress that can prevail in that point is the lowest of all points in the material. If the strain increases with time, there will be a time instant where this weakest point will start following the softening part of the stress-strain curve, so that the stress in that point decreases, while the strain increases. Due to equilibrium requirements, the stress in the neighbouring points has to decrease too, but these points are still on the hardening part of the curve, so the strain in these points will decrease. The weakest point thus takes all the deformation of the material, while the rest of the body returns to its initial state: a localization zone has occurred.

As an example, a MLFEM calculation on a beam consisting of three bilinear quadrilateral elements is carried out (cf. Fig. 3). The left hand side of the beam is clamped, while the other end is displaced. In each of the four integration points of the elements, the stresses, and their derivatives with respect to the strains, are calculated in the above mentioned way, by carrying out finite element calculations on an RVE, for which the mesh is plotted in Fig. 3d. The regions marked by the thick drawn lines are again interface regions; the other ones are linear elastic isotropic material bodies. Due to the interfaces, the relation (6) for the RVE is a strain-softening one. The second element is the weakest: the maximal stress that can prevail in that element is 20% smaller than that of the other two elements.

The force F_x at the right end is plotted in Fig. 3e as a function of the displacement u_x. We see that this force decreases beyond a certain displacement. Fig. 3a shows the initial configuration, and in Figs. 3b and 3c two deformed configuration are depicted. The one in Fig. 3b is taken at the point where F_x is maximal, while the one in Fig. 3c is taken at the final displacement, when the force has decreased.

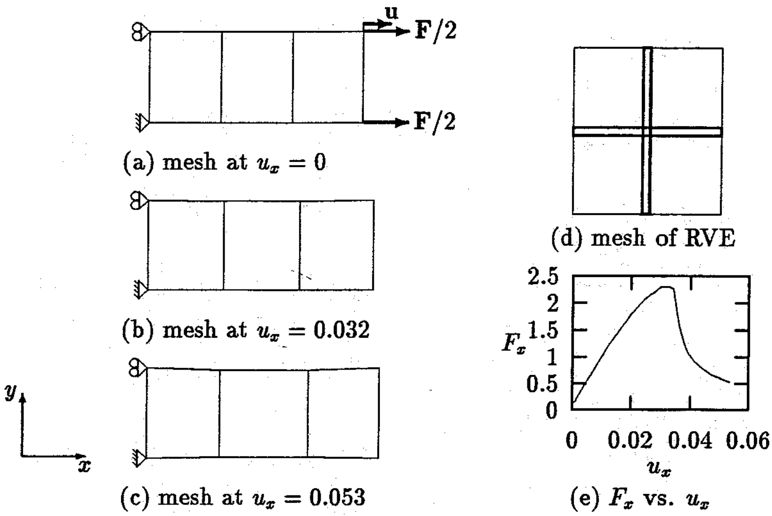


Figure 3 Three configurations of a beam consisting of three bilinear quadrilateral elements (a–c), in which in each of the four integration points four micromechanical calculations are carried out on a fixed mesh of the RVE depicted in (d). The force F_x on the boundary is plotted as a function of the displacement u_x of that boundary in (e).

We see that the second element indeed takes all the deformation, while the other two elements return to their initial states. Hence, if we use a normal finite element method to calculate the response behaviour of the material, one of the elements in the mesh is the weakest, so that the localization zone is confined to one element. Thus, the response behaviour depends upon the finite element mesh (see also [1]).

In order to solve this, we need a nonlocal or gradient dependent formulation of the constitutive equation (6) (cf. [2]). A nonlocal relation can be obtained, by considering with each point $\mathbf{x}_0$ of the fictitious material body a cube $\Omega(\mathbf{x}_0) = \{\mathbf{x} \mid |x_i - x_{0i}| < r,\ i = 1,2,3\}$, and by taking the mean of (6) over $\Omega(\mathbf{x}_0)$. Setting $\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\xi}$, and expanding the integrands into Taylor series around $\mathbf{x}_0$, we obtain a gradient dependent formulation of (6),

$$\bar{\sigma} + \frac{r^2}{6}\Delta\bar{\sigma} = \mathbf{G}(\mathbf{x}, \bar{\varepsilon}) + \frac{r^2}{6}\mathbf{H}(\mathbf{x}, \operatorname{grad}\bar{\varepsilon}, \Delta\bar{\varepsilon}) + O(r^4), \quad r \to 0, \tag{8}$$

where Δ is the Laplace operator with respect to $\mathbf{x}$, and where $\mathbf{H}$ contains only derivatives of $\mathbf{G}$, and is quadratic in $\operatorname{grad}\bar{\varepsilon}$ and linear in $\Delta\bar{\varepsilon}$.

If we use one these relations in a finite element analysis, the solution becomes independent of the mesh [2]. However, both these relations contain the unknown length parameter r. This parameter is related to the width of the localization zone. It has to be determined by comparing the results of finite element calculations based on the micromechanical model for a regular stack of RVEs (cf. Fig. 2), with those based on the nonlocal or gradient formulation of the homogenized model for that stack, and by varying the number of RVEs in that stack.

4 Conclusions

Starting with a micromechanical model for a composite, in which the components are assumed to obey continuum laws, and with a model for the interaction between two contiguous components, we formulated a (formal) macroscopic constitutive equation by relating the average of the stress field in a representative volume element to the average strain imposed on that RVE. The averaging has to be done numerically (using parameter estimation methods), since the RVE shows a strain-softening behaviour.

The strain-softening of the RVE leads, in addition, to numerical problems with the finite element method applied to the local form of the homogenized constitutive equation, since the solution will be mesh-dependent. These problems can be solved by using a nonlocal, or gradient dependent formulation of the constitutive equation.

The internal length parameter that appears in the nonlocal, and gradient formulations, has to be determined by comparing micromechanical calculations to calculations on the macroscopic continuum.

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