Efficacy of homogenization techniques for locally periodic composites

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SUMMARY. The aim of the present paper is to analyze the accuracy of macroscopic constitutive properties obtained by using homogenization based techniques, to represent the failure properties of locally periodic defected composites. To this end a numerical investigation based on a finite element formulation in conjunction with an interface model is here carried out to obtain the homogenized constitutive properties of a composite solid in the context of deformation controlled micro-structures. A novel homogenization computational scheme is introduced to compute energy release rate values at crack tips inside each unit cell for the composite structure and interfacial stresses, from results of the homogenized analysis.
With reference to a 2D composite structure composed of a regular and finite assembly of unit cells, comparisons in terms of energy release rate and fiber/matrix interface stresses between results obtained by means of direct analysis, which recognizes explicitly the composite microstructure, and those computed by using the homogenized properties of the composite, are developed. Both the cases of a debonded and a perfectly bonded fiber-reinforced microstructure are studied.

1 INTRODUCTION

The prediction of macroscopic properties is a problem of great importance in the study of composite materials. As a matter of fact, a precise description of microstructural details, such as fibers, matrix, interfaces, voids, may involve a large computational cost. Several methodologies have been formulated able to determine the macroscopic response of a heterogeneous composite material with elastic micro-constituent [1]. These methods are often applied in conjunction with finite element methodologies. The transition from the micro-to-macro scale is called homogenization. Generally speaking, the homogenized analysis of a composite solid is performed by means of two decoupled problems in cascade. In the first one the micro-structural details are modeled to determine the global response of a representative volume element (RVE) of the composite microstructure. These properties are then utilized in the second problem, called macro-problem, in which the composite structure is replaced by an equivalent homogeneous material.

In many cases damage phenomena may occur at the microscopic level, such as void growth, micro-crack, imperfect bond between different phases. These damage mechanisms affect seriously the macroscopic behavior of the composite materials [2,-4]. Moreover, for many practical cases perfect periodicity does not hold, and the composite material can be often only locally periodic, i.e. the ratio of the micro-scale length to the macroscale length is significantly larger than zero [5-7]. Consequently, the analysis of the accuracy of macroscopic constitutive properties obtained by using homogenization based techniques, to represent the failure properties of locally periodic defected composites, plays a relevant role.

To this end a numerical investigation based on a finite element formulation in conjunction with an interface model is here carried out to obtain the homogenized constitutive properties of a composite solid in the context of deformation controlled micro-structures. The micro to macro transition is performed by adopting periodic boundary conditions. Therefore, in order to assess the accuracy of the proposed homogenized procedure, the obtained macroscopic properties are applied to the study of a 2D composite structure composed of a regular and finite assembly of unit cells. Global boundary conditions involve a non uniform macroscopic deformation gradient and both the cases of a debonded and a perfectly bonded fiber-reinforced microstructure are studied. Comparisons in terms of energy release rate and fiber/matrix interface stresses between results obtained by means of direct analysis, which recognizes explicitly the composite microstructure, and those computed by using the homogenized properties of the composite, are developed. A novel homogenization computational scheme is introduced to compute energy release rate values at crack tips inside each unit cell for the composite structure and interfacial stresses, from results of the homogenized analysis. The computational scheme adopts a *J*-integral formulation established for composite micro-structures, able to determine the energy release rate at the crack tip when micro-cracking and contact within the constituents or at the interface between the composite micro-constituents occur.

2 MACROSCOPIC PROPERTIES

Let us consider that the representative volume element (RVE) of a periodic composite microstructure, denoted by V, consists of a solid portion S and a hole portion H, namely $V=S\cup H$, and the latter part is assume to include microscopic discontinuities (cracks and interface debonding) and/or cavities, such that ∂H represents the union of micro-crack and micro-void surfaces. The microscopic displacement field can be expressed as the sum of a linear part $\bar{\boldsymbol{\varepsilon}}\boldsymbol{x}$ and a periodic fluctuation field $\boldsymbol{w}$:

$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}}\boldsymbol{x} + \boldsymbol{w}(\boldsymbol{x}), \quad \bar{\boldsymbol{\varepsilon}} = \frac{1}{|V|}\int_{\partial V} \boldsymbol{u} \otimes_s \boldsymbol{n} dA \ , \tag{1}$$

where $\otimes_s$ is the symmetric part the tensor product $\otimes$ and $\boldsymbol{n}$ denotes the outward normal at $\boldsymbol{x}\in\partial V$.

The microscopic constitutive response of the composite material is assumed linearly hyperelastic and the microscopic strain energy is assumed convex. The homogenization condition can be obtained by means of the following minimization problem:

$$\bar{W}(\bar{\boldsymbol{\varepsilon}}) = \inf_{\boldsymbol{w}\in A(\bar{\boldsymbol{\varepsilon}})} \frac{1}{|V|}\int_{S} W\left(\boldsymbol{\varepsilon}(\boldsymbol{w}) = \bar{\boldsymbol{\varepsilon}}\boldsymbol{x} + \nabla_s \boldsymbol{w}, \boldsymbol{x}\right) dV \ , \tag{2}$$

where $\boldsymbol{w} \in A(\bar{\boldsymbol{\varepsilon}})$ denotes admissible fluctuation fields satisfying the periodicity constraints on the boundary ∂V. The minimization principle provides the macro-stress potential as the minimum volume average of the microscopic strain energy W with respect to admissible fluctuation fields $\boldsymbol{w} \in A(\bar{\boldsymbol{\varepsilon}})$. The macro-stress and macroscopic moduli tensor are defined in terms of the first and second derivatives of the macro-stress potential with respect to the macro-strain:

$$\bar{\boldsymbol{\sigma}} = \frac{\partial \bar{W}}{\partial \bar{\boldsymbol{\varepsilon}}} = \frac{1}{|V|}\int_{\partial V} \boldsymbol{t} \otimes \boldsymbol{n} dA, \quad \bar{\boldsymbol{C}} = \frac{\partial^2 \bar{W}}{\partial \bar{\boldsymbol{\varepsilon}}^2} \ , \tag{3}$$

where $\boldsymbol{t}$ is the traction field. In presence of unilateral frictionless contact at the debonded interfaces or micro-cracks surfaces, the minimum principle must be appropriately modified in order to incorporate the kinematical unilateral contact condition and leads to a variational inequality. When unilateral frictionless contact occurs the macroscopic constitutive behavior of the composite turns out to be nonlinear but remains hyperelastic (rate- and path- independent). In fact, the contact area is not known a-priori but depends only on the direction of the prescribed macro-strain, $\hat{\bar{\varepsilon}}=\bar{\varepsilon}/\|\bar{\varepsilon}\|$, and this implies that the tensor of macroscopic moduli $\bar{\boldsymbol{C}}=\bar{\boldsymbol{C}}(\bar{\varepsilon})$ (Eq. $(3)_2$ is here intended as second Gateaux derivative when it exists) satisfies $\bar{\boldsymbol{C}}(\lambda\bar{\varepsilon})=\bar{\boldsymbol{C}}(\bar{\varepsilon})$ for every strictly positive real number λ (see [5] for additional details).

The macroscopic tangent moduli with respect to the macro-strain when the damage configuration remains unchanged, can be computed by eqn (3) and depends on the crack length l and on the macro-strain direction $\hat{\bar{\boldsymbol{\varepsilon}}} = \bar{\boldsymbol{\varepsilon}}/\|\bar{\boldsymbol{\varepsilon}}\|$ owing to non-linearities introduced by contact. As a consequence the macroscopic constitutive law can be written as:

$$\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{C}}\left(\hat{\bar{\boldsymbol{\varepsilon}}}, l\right)\bar{\boldsymbol{\varepsilon}} . \tag{4}$$

Crack propagation is predicted by means of the classical fracture mechanics criterion:

$$\boldsymbol{G}\left(\bar{\boldsymbol{\varepsilon}}, l\right) = \boldsymbol{G}_C \Rightarrow \dot{l} \geq 0 \tag{5}$$

where G is the energy release rate associated with the crack length l and G_c is the fracture toughness of the material. When the non-linear damage evolution relation between the prescribed macro-strain and the crack length $l=l\left(\bar{\boldsymbol{\varepsilon}}\right)$ extracted from eqn (5), is introduced in eqn (4) the macroscopic stress-strain relation becomes highly non-linear and depends strongly on the macro-strain history.

The energy release rate G for a given damage configuration and a prescribed macro-strain, is calculated by means of the J-integral technique. In the general case when the crack is not straight and material interfaces inside the region R individuated by an arbitrary path Γ, surrounding the crack tip which begins and ends on the crack faces, ∂D_δ and the two faces of the crack are not aligned with the direction of propagation $\boldsymbol{e}$, the following expression can be established:

$$\begin{aligned} G\left(\bar{\boldsymbol{\varepsilon}}, l\right) &= \lim_{\delta\to 0} J\left(\partial D_\delta, \bar{\boldsymbol{\varepsilon}}, l\right) = \lim_{\delta\to 0} \boldsymbol{e}\bullet \int_{\partial D_\delta} \left(W\boldsymbol{n} - \nabla \boldsymbol{u}^T \boldsymbol{\sigma}\boldsymbol{n}\right) ds = \lim_{\delta\to 0} \boldsymbol{e}\bullet \left[\int_{\Gamma} \left(W\boldsymbol{n} - \nabla \boldsymbol{u}^T \boldsymbol{\sigma}\boldsymbol{n}\right) ds + \right. \\ &\left. \int_{\Gamma_c} \left[\!\left[W\boldsymbol{1} - \nabla \boldsymbol{u}^T \boldsymbol{\sigma} \right]\!\right] \boldsymbol{m} ds + \int_{\gamma} \left[\!\left[W\boldsymbol{1} - \nabla \boldsymbol{u}^T \boldsymbol{\sigma} \right]\!\right] \boldsymbol{q} ds \right] \end{aligned} , \tag{6}$$

where D_δ is a disc of radius δ centered at the crack tip, $\boldsymbol{n}$ is the unit outward normal to ∂D_δ, γ denotes the union of the material interfaces, $\boldsymbol{n}$ is the unit outward normal to ∂D_δ or Γ, $\boldsymbol{m}$ is the normal to crack faces Γ_c, $\boldsymbol{q}$ is the normal to material interface and the double brackets indicate the jump of the enclosed quantity evaluated as the difference between the values from the negative and positive sides of the material interface. It must be noted that the second contribution to the second integral vanishes only when contact does not occur. Moreover, it can be observed that near the crack tip the contribution from the second integral approaches zero since the crack face normal becomes perpendicular to the crack propagation direction. This avoids difficulties in the numerical evaluation of jump quantities near the crack tip owing to stress singularities.

3 NUMERICAL RESULTS

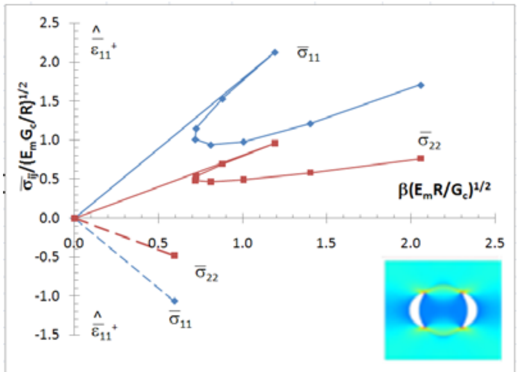
An interface model has been developed in order to deal with crack growth and unilateral frictionless contact between crack faces. The model is formulated by means of a penalty stiffness parameter *k* dependent on the spatial coordinate, and a crack parameter *d*, assuming the value 1 in the cracked region and 0 in the uncracked one. A continuation strategy is used by carrying out a parametric analysis with respect to *k*. The variational problem of homogeneization was discretized by means of a displacement-type finite element (FE) approximation implemented by using the commercial software COMSOL MULTIPHISYCS^{TM} and a non linear solution strategy was adopted to deal with contact, based on the damped Newton method. Periodic boundary conditions were implemented in the homogenization procedure by means of the extrusion coupling variable methodology, according to which the displacement field is made available on the opposite boundary faces of the RVE.

Tangent moduli $\bar{\boldsymbol{C}}_{ijhk}\left(l,\hat{\bar{\varepsilon}}\right)$ were calculated with reference to the initial unstressed configuration by imposing the constraint condition for the relative displacement in the normal direction to the contact interface, along the contact zone associated with the given macro-strain. The contact zone can be obtained by solving the boundary value problem for the RVE driven by the macro-strain direction $\hat{\bar{\varepsilon}}$, since it depends only on the macro-strain direction. The energy release rate was determined by using integration coupling variables.

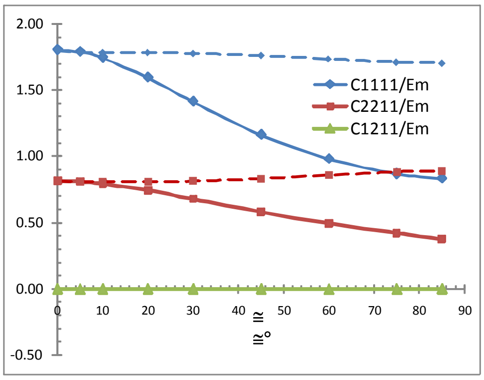
3.1 *Macroscopic constitutive law for a debonded fiber reinforced composite*

A 2D debonded fiber-reinforced composite is here analyzed. A squared RVE is assumed, composed of a matrix including a centered circular fiber. The side length of the RVE is h=1.0*mm*, the diameter of the fiber d=0.5h. The material constants are E_m=2 GPa, ν_m=0.33, for the matrix, and E_f=10 E_m, ν_f=0.20, for the fiber. It is assumed that two interface cracks of length l can grow symmetrically and the fiber is perfectly bonded to the matrix except over the region defined by $|\theta|\leq\bar{\theta}$ and $|\pi-\theta|\leq\bar{\theta}$ where $\bar{\theta}$ is one half the angle subtended by each symmetric interface crack. Plane strain conditions are assumed. Numerical results for macroscopic constitutive laws were computed with reference to a small initial relative crack length l_0/h, equal to 0.022.

The assumed macro-strain path direction is a uniaxial mode in the x_1 direction, $\hat{\bar{\boldsymbol{\varepsilon}}}_1^{\pm}=\pm\,\boldsymbol{e}_1\otimes\boldsymbol{e}_1$, where superscript $\pm$ denotes the positive or negative macro-strain path direction. Results demonstrate that for the positive direction of the uniaxial deformation mode $\hat{\bar{\boldsymbol{\varepsilon}}}_1^{+}$ crack faces do not overlap. On the contrary, for the compressive uniaxial deformation mode $\hat{\bar{\boldsymbol{\varepsilon}}}_1^{-}$, the cracks are completely closed. Finally, it must be observed that due to symmetry the energy release rate takes the same value at all crack tips. The macroscopic stress-strain law for the uniaxial macro-strain path is illustrated in Fig.1. The initial behaviour of the macroscopic constitutive laws is linear and characterized by the moduli $\bar{\boldsymbol{C}}\left(l_0\right)$ computed with reference to the initial crack length l_0. Since for the compression mode, the energy release rates at crack tips are negligible, due to the fact that cracks are completely closed, the behavior is indefinitely linear elastic being characterized by the undamaged moduli $\bar{\boldsymbol{C}}\left(l=l_0\right)$ and cracks do not propagate. This behavior is denoted by a dashed line in Fig. 1a. On the contrary, for the positive macro-strain direction, energy release rate is not negligible and interface cracks propagate and the macroscopic constitutive laws show a snap-through behavior. Fig. 1b shows the behavior of macroscopic moduli both in tension (continuous line) and in compression (dashed line). It can be noted that, due to contact, in compression macroscopic moduli are scarcely influenced by the crack angle.



a)



b)

Figure 1: Macroscopic dimensionless macro-stresses versus macroscopic strain parameter for the x_1 uniaxial macro-strain path (a); Behavior of the macroscopic moduli as the crack angle increases (b).

3.2 *Homogenized and direct analysis.*

A 2D composite structure composed of a regular and finite assembly of locally defected unit cells subjected to mixed boundary conditions of traction and place, is studied in order to analyze the effectiveness of the homogenization procedure to capture microscopic properties governing the failure behavior of a composite. Two kinds of microstructure are examined, namely a debonded fiber reinforced composite with a symmetric debonding characterized by $\overline{\theta} = \pi / 4$ and a perfectly bonded fiber reinforced composite. In the former case, comparisons between energy release rate values obtained by means of direct analysis, recognizing explicitly all microstructural details, of a 2D composite structure, composed by a regular arrangement of 5x5 unit cells, and those computed by means of a microscopic analysis of a single RVE, driven by the imposed macro-strain as obtained from a macroscopic analysis of the homogenized macro-element, are carried out. In the latter case, comparisons between the direct analysis and the homogenized one are made in terms of normal and tangential interface stresses. Plane strain conditions are assumed.

A computational procedure is here proposed to compute energy release rate and interface stresses values at crack tips inside each unit cell for the composite structure from results of the homogenized analysis. The computational procedure can be accomplished according to the following steps:

1) *Calculation* of the homogenized moduli by using a single RVE;

2) *Analysis* of the composite structure adopting the homogenized moduli obtained in the previous step;

3) *Determination* of macro-strain by Eq. $(1)_2$ for each unit cell using displacements obtained in the previous step and performing the integration with reference to the external boundary of the unit cell;

3) *Evaluation* of the local quantities (energy release rate, interface stresses) inside each unit cell of the locally periodic arrangement, by imposing the previously computed macro-strain on the unit cell.

When contact occurs the procedure becomes more complex, since it must takes into account for the dependence on the macro-strain direction, which can vary from cell to cell, of the homogenized moduli tensor. In this case for each unit cell an average macro-strain direction is computed over the external unit cell boundary by an iterative procedure and the contact configuration determined by using this macro-strain direction can be assumed to represent the contact situation inside each cell of the locally periodic composite in an average sense (see [5] for additional details).

3.3 .1 *Debonded microstructure.*

This application involves a 2D composite structure subjected to an imposed displacement in the *x*-direction Δ equal to 5*h*/1000 at its right side and is fixed at its left one, while it is traction free at the upper and lower sides. The composite structure in the direct analysis is discretized by means of an unstructured mesh of quadratic triangular elements and appropriate mesh refinement along the contours used for the *J*-integral evaluation at each crack tip are included. Fig. 2 shows the mesh adopted in the analysis which is arranged in 191,832 triangular elements resulting in 216,495 degrees of freedom.

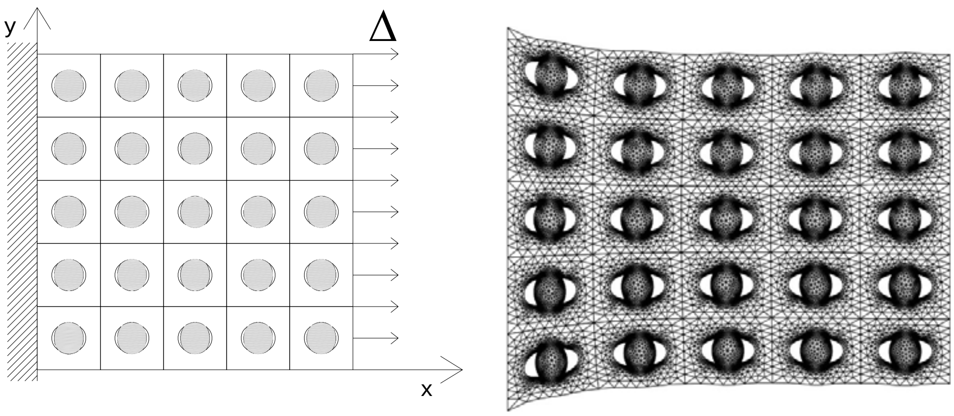


Figure 2: Debonded fiber reinforced composite: geometry (left) and deformed mesh (right).

In this boundary value problem crack faces never come into contact. Fig. 3 shows the variation with the position of the crack tip of the dimensionless energy release rate values in the direct analysis. Owing to symmetry, only one half of the composite structure is considered in the results shown in Fig. 3. The expression used for the dimensionless energy release rate is $\bar{G} = E_m \Delta^2 l(1-\upsilon_m{}^2)/H^2$ where *H* is the total height of the composite structure is equal to 5*h*. The origin of the co-ordinate system is placed in the lower left corner of the composite structure. Results show a large variation of energy release rate in proximity of the fixed end.

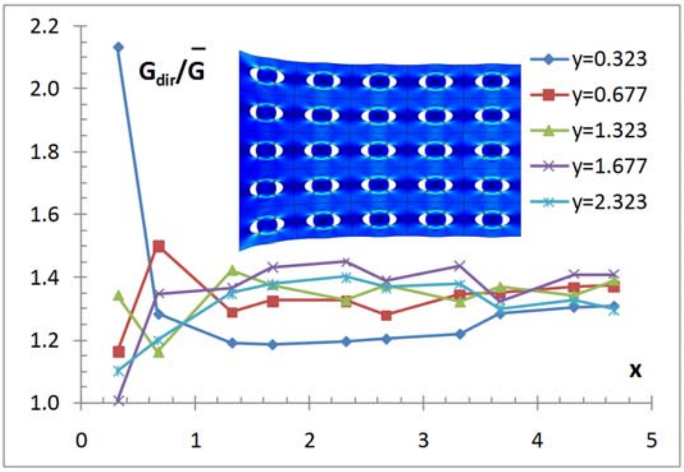


Figure 3: Variation of the energy release rate with the position of crack tip.

Fig. 4 shows the relative percentage error *e%* in energy release rate at each crack tip evaluated as $\left(G_{dir} - G_{hom}\right)/G_{dir} x100$, where G_{dir} and G_{hom} are respectively the energy release rate values in the direct and homogenized analyses. The error analysis shows that generally the largest relative percentage absolute error |e%| is 29.20%. Due to boundary layer effects the largest errors along the lines parallel to the y-axis generally are attained near the fixed end (x=0.32h, x=0.68h). In particular, along the line x=0.32h the largest error is attained for the external cells (namely for crack tips located at x=0.32h, y=0.32h and x=0.32h, y=4.48h) with an underestimation of about 29.20%. The smallest relative percentage absolute error |e%| is equal to 0.01% for the crack tips located at x=4.32h and y=1.32, 3.68. Away from the boundaries, at a distance of one half the unit cell, the absolute errors become much smaller and lower than about 6.79%.

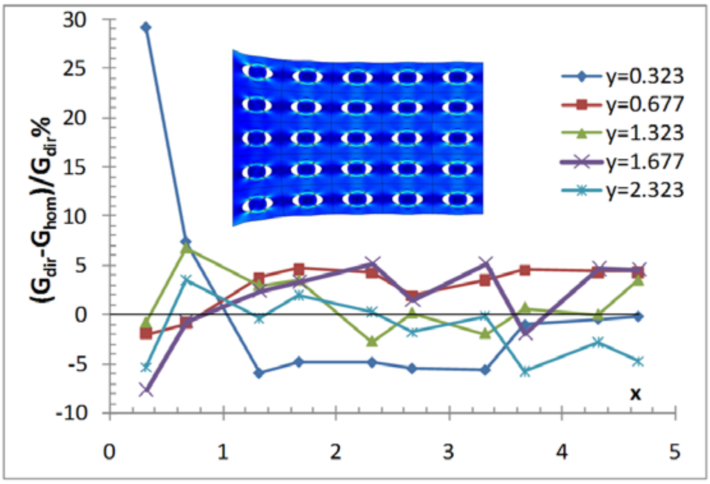


Figure 4: Percentage errors between homogenized and direct analyses in terms of energy release rate.

3.3.2 *Perfectly bonded microstructure*

The second application is devoted to a perfectly bonded microstructure and is characterized by the same boundary value problem considered in the previous example. Fig. 5 shows the mesh adopted in the analysis which is arranged in 88,320 triangular elements resulting in 354,125 degrees of freedom.

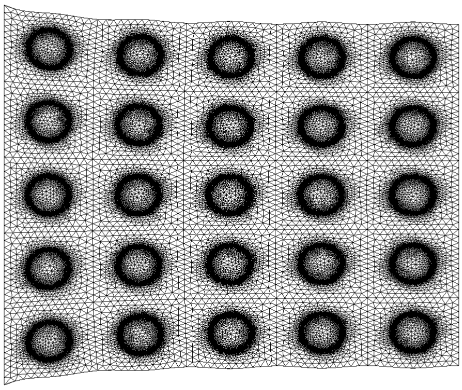


Figure 5: Perfectly bonded fiber reinforced composite: deformed mesh.

Figs 6 and 7 show the distribution of dimensionless interfacial stresses as computed by the direct (continuous line) and the homogenized (dashed line) procedures in the lower left and the middle unit cells, respectively. Since failure in composites is usually correlated to interfacial stresses, it is of notable importance to consider these quantities. Numerical calculations have shown that interfacial stresses are always underestimated by the homogenized analysis. The maximum relative percentage errors for the normal interface stresses are 25% and 25.4% for the lower left and middle cells, respectively. In the case of the tangential interface stresses the largest errors are 28.3% and 29.7% for the lower left and middle cells.

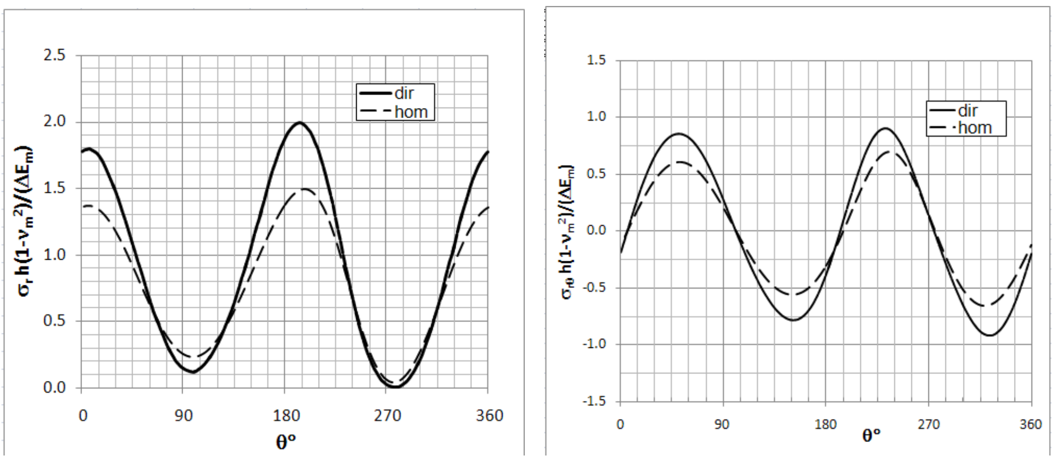


Figure 6: Comparisons in terms of normal and tangential interface stresses between the homogenized and direct analyses. Lower left unit cell.

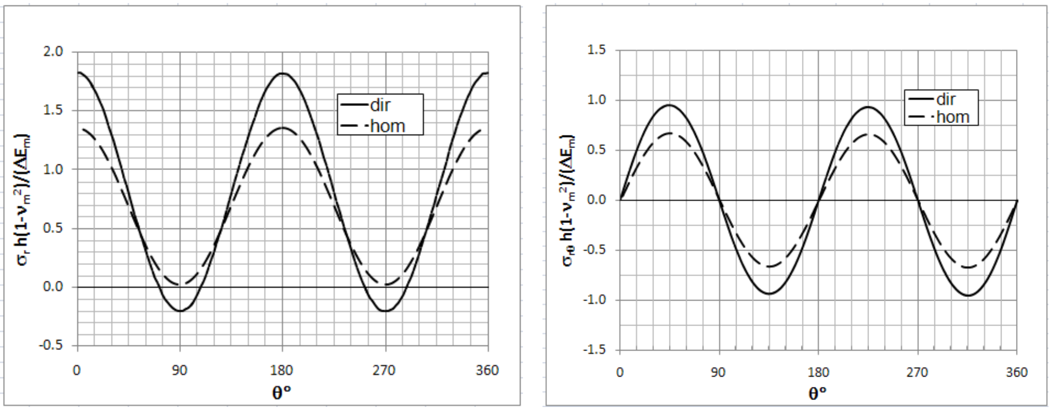


Figure 7: Comparisons in terms of normal and tangential interface stresses between the homogenized and direct analyses. Middle unit cell.

4 CONCLUSIONS

The effects of micro-cracking evolution and unilateral frictionless contact on the macroscopic constitutive properties of elastic composite materials and the accuracy of the macroscopic constitutive properties to represent the failure properties of locally periodic defected composites are investigated. These aspects are of notable significance in the context of the homogenization theory of composite materials containing microscopic defects, such as micro-cracks and interface cracks. An original micro-mechanical model is proposed based on homogenization techniques, fracture mechanics concepts and interface models. Non-linear macroscopic constitutive laws are determined by taking into account the evolution in micro-structural configuration due to crack growth and crack-face contact interaction along uniaxial and shear macro-strain paths. Numerical applications are carried out by coupling a finite element formulation and an interface model, with reference to two typical 2D micro-structures, namely a debonded and a perfectly bonded fiber-reinforced microstructure. Results point out the highly non-linearity of the macroscopic law and very strong dependence of the macroscopic constitutive law for a microstructure with evolving defects, on the macro-strain path.

In order to estimate the accuracy of the obtained macroscopic constitutive properties to represent the failure characteristics of locally periodic defected composites, comparisons in terms of energy release rate and fiber/matrix interface stresses between results obtained by means of direct analysis, which recognizes explicitly the composite microstructure, and those computed by using the homogenized properties of the composite, are developed. To this end an homogenization computational scheme is introduced to compute local quantities inside each unit cell for the composite structure, from results of the homogenized analysis. The examined composite structure is composed of a regular arrangement of 5x5 unit cells and adopts the above described two micro-structures.

The obtained results show the capability of the proposed model to provide a macroscopic constitutive law incorporating the influence of evolving defects at the micro-structural level and to capture failure mechanisms associated with micro-cracking and contact. On the other hand, these results evidence the limitations introduced by the proposed model when practical composite structure problems must be solved.

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