On a numerical DEM-based approach for assessing thermoelastic properties of composite materials

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ABSTRACT

The present contribution is dedicated to a Discrete Element Method (DEM)-based approach aiming at assessing the thermomechanical behavior of composite materials. Such an approach presents several advantages in comparison to other classical methods as the Finite Element (FE) one. This enables a better description of the multi-scale behavior of the material with the inherent variability related to the microscopic scale. It also gives the possibility to directly access information such strain and stress fields and heat flux density at the scale of the discrete element. In the current work, a focus is done on the thermoelastic properties of a heterogeneous medium composed of a single inclusion. A 2D representative pattern is generated and discretized using a granular packing composed of cylindrical particles in contact point. This is generated using a process based on the Lubachevsky-Stillinger Algorithm (LSA) coupled to a DEM approach based on a smooth formulation. A hybrid-particulate model is considered to model the mechanical behavior of the material. In this approach, the contact between two particles is described by a beam element which models the cohesive link at the microscopic scale. Heat transfer is simulated using an iterative time-dependent scheme based on the Fourier's law and Voronoï's mosaics generated from granular packings. A full range of thermoelastic properties are considered in order to investigate several configurations of material from an insulative fibre less resilient than the surrounding matrix to a conductive fibre more resilient than the matrix. Estimated properties are compared to those obtained from other numerical methods such as FE and Fast Fourier Transform (FFT)-based calculations and analytical models. Results highlight the ability of the proposed approach to estimate effective thermoelastic properties. These first results pave the way of interesting insights since taking into account non-linear behaviors, interfacial effects and damaging in the proposed approach can be envisaged in a next future.

Keywords: Discrete element method, Multi-scale approach, Composite material, Thermoelastic properties, Equivalent continuous domain.

Introduction

Composite materials arouse the interest of many industrial sectors such as aeronautic, aerospace, automotive, building and marine. These are indeed characterized by excellent stiffness-to-weight and thermal conductivity-to-weight ratios which make them adaptable to different situations and make them able to serve specific purposes and exhibit desirable thermomechanical properties. Besides, the development of biocomposites composed of natural fibres as flax or hemp show their ability to respond to current environnement issues as the reduction of gas emissions. Research to increase performance and safety of composites pieces in many fields requires the development of means of investigation concerning the behavior in service and durability of materials. Durability characterizes the ability of the material to resist to degradation of the thermomechanical properties over time under various types of sollicitations. The scientific challenge therefore consists in developing reliable numerical methods for achieving a better extrapolation of the multi-scale thermomechanical behavior of the composite as well as a better description of various phenomena arising in the material such as crack initiations, debonding effects, local variability and heterogeneity.

Considered as an alternative to the classical FE method, the DEM is an ideal tool for solving mechanical problems in which multiple scales and discontinuities arise. Indeed, DEM is characterized by a good description of microscopic phenomena, an easy treatment of complex structures and a very fine time scale which enables to describe the local behavior of a large number of particles. Among the early studies, DEM was used to explore and gain new insights into various physical applications from geomechanics applications [1, 2] to tribological simulation approaches [3, 4] and heat transfert simulation in multi-contact systems [5, 6]. More recently, André et al. [7] and Haddad et al. [8] considered a hybrid particulate-lattice model in which particles are linked using cohesive beam elements. Thus, the DEM was made able to quantitatively model the mechanical behavior of homogeneous and heterogeneous materials as well as fracture phenomena as crack formation and propagation.

The present work is dedicated to an extension of the hybrid particulate-lattice model to the characterization of thermoelastic behavior of composite materials. The main objective is to highlight the ability of a DEM-based approach to the assessment of thermoelastic properties such as the thermal conductivity and the Young's modulus. For this purpose, a focus is done on a heterogeneous medium composed of a single inclusion. A 2D square-shaped representative pattern is modeled and discretized by a granular packing composed of cylindrical particles in contact point generated with the help of an efficient process based on the LSA [9] coupled to a DEM approach using a smooth formulation. In order to take into account in the same time the elastic behavior and the heat transfer within the material, the initial set of contacts is densified by a Delaunay triangulation process performed from this initial cloud of particle's centers. It leads to a better description of the heterogeneous medium and more accurate results by the hybrid-particulate model. Besides, a Voronoï mosaic is associated to the Delaunay triangulation which provides in the same time a representative volume and transmission contact surfaces to each particle. Thus, the heat transfer by conduction can be simulated using an iterative time-dependent scheme based on the Fourier's law where representative volumes and surfaces come from the Voronoï mosaic.

This paper is organized as follows. First, we describe the heat transfer scheme and the hybrid-particulate approach for simulating the thermoelastic behavior of the material. Second, the numerical model is validated in the context of a homogeneous material. Thermal and boundary conditions are imposed to the 2D square pattern in order to reproduce simple tests as tensile and shear ones leading to thermoelastic properties. Finally, the DEM-based approach is applied to the case of a single circular inclusion embedded in a matrix. For validation purposes, a large range of material configurations are investigated from an insulative fibre less resilient than the surrounding matrix to a conductive fibre more resilient than the matrix. Comparisons are carried out with several numerical methods, namely FE and FFT-based calculations and analytical models.

Numerical model

Equivalent Continuous Domain

The first step of the proposed DEM-based approach consists in discretizing the continuous domain at the macroscopic scale by a granular packing composed of cylindrical particles in 2D. The generation of the granular packing is done by the efficient LSA coupled to the DEM using a smooth formulation. The idea is that the early stages of the LSA are dominated by the densification of the system and consequently more efficiently performed than the last steps where the number of contacts dramatically increases. In the coupled approach, the last steps are performed by the DEM using a smooth formulation which is more suited to control the multiplicity of contacts than the LSA. Under several assumptions of polydispersity, orientation and size, the granular domain can be considered as an Equivalent Continuous Domain (ECD) in that this is enough representative of the continuous medium. First, the compacity of the granular domain has to be closed to 0.85 which corresponds to the Random Close Packing (RCP) for a random granular packing composed of cylindrical particles in 2D. Second, the coordination number which represents the average number of particles in contact with one given particle has to be close to 4.5. Third, a slight polydispersity of particle size must be introduced in order to avoid undesirable directional effects. Typically, the particle's radius follows a Gaussian distribution law and the dispersion is characterized by the coefficient of variation which is the ratio between the standard deviation and the average radius. For information purposes, this is set to 0.3 in the present work. These three first parameters ensure the randomness of the granular packing and consequently the isotropy of the ECD. In other words, this ensures that thermoelastic properties are independent of the direction. At last, the number of particles represents the fineness of the discretized medium in a similar way to a FE Mesh. As done by previous authors, the network of contacts is finally densified using a Delaunay triangulation process applied from this initial cloud of particle's centers. Thus, the coordination number comes from about 4.5 to about 5.9 and about 10% of new contacts are generated. A Voronoï tessellation is finally associated to the Delaunay triangulation. This provides in the same time an area of representation for each particle and its contacts. Such a process turns out to be not costly in computational time as long as dynamic effects are not considered since the remeshing process is then not required.

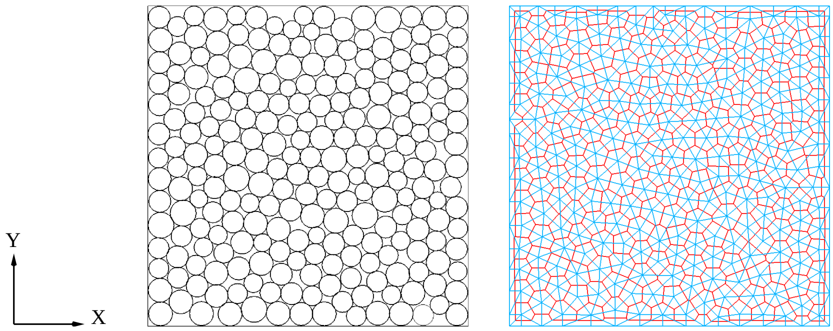

Figure 1. Example of a typical 2D Voronoï construction based on a granular packing constituted of 200 particles: granular packing (a) and corresponding Voronoï tessellation (b)

Heat transfer by conduction

In the present model, each particle i is related to a Voronoï cell considered as its representative element (Fig. 2). This polygon has a number of sides equal to the number of particles j in contact with the particle i. The heat flux transmitted by the contact surface between two particles i, j is defined as follows:

$$W_{ij} = H_c^{i,j}(T_j - T_i) \tag{1}$$

where T_i, T_j are the temperatures of particles i, j and $H_c^{i,j}$ is the coefficient of thermal conductance: $H_c^{i,j} = \frac{S_{ij}^t k}{d_{ij}}$, with λ the conductivity of material, d_{ij} the distance between the centers of particles i, j and S_{ij}^t the area of heat transmission surface related to the corresponding polygon side.

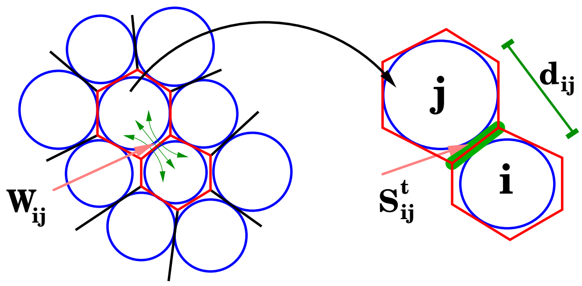

Figure 2. Definition of the heat transmission surface S_{ij}^t

The corresponding equation of heat transfer is expressed for each particle i by:

$$C_i^d \frac{dT_i}{dt} + \sum_{j=1}^{n_i} W_{ij} = Q_i \tag{2}$$

where Q_i represents the external heat flux associated to the particle i and n_i is the number of neighbors of particle i. C_i^d is the heat capacity of the particle given by:

$$C_i^d = c_p \rho_d V_i \tag{3}$$

with V_i and ρ_d are the volume and the density of the particle respectively and c_p is the specific heat of constitutive material. For the purpose of conservation mass, the discrete element mass is adjusted to the polygon one. To satisfy this assumption, we consider ρ_c as the constitutive material density, ρ_d is then connected to ρ_c through the following relationship:

$$\rho_d = \frac{V_{poly}}{V_i} \rho_c \tag{4}$$

where V_{poly} is the polygon's volume. The discretization of equation for heat transfer (2) in time leads to:

$$T_i^{t+\Delta t} = T_i^t + \frac{\Delta t}{c_p \rho_d V_i} \underbrace{[Q_i + \sum_{j=1}^{n_i} \frac{S_{ij}^t \lambda}{d_{ij}} (T_j^t - T_i^t)]}_{Q_i^{tot}} \tag{5}$$

Elastic behavior

We consider a hybrid particulate-lattice model in which the interaction between two cylindrical particles in contact is modeled by a beam of length L_μ, Young's modulus E_μ, cross-section A_μ and quadratic moment I_μ (Fig.3). Therefore, the cohesive contacts are maintained by a vector of three-component generalized forces acting as internal forces. The normal component acts as an attractive force, the tangential component allows to resist to the tangential relative displacement and the moment component counteracts the bending motion [7].

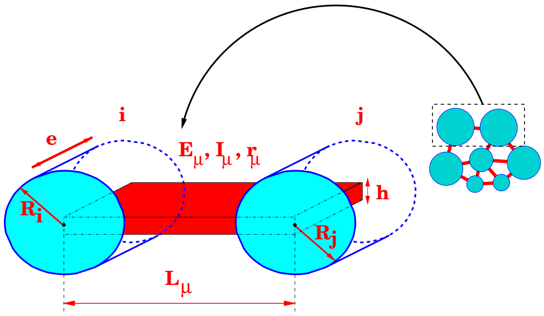

Figure 3. Hybrid particulate-lattice model

The cross-section A_μ is rectangular with sides e and h, where e is the thickness of the granular medium and h is the height of the cross section defined by:

$$h = r_\mu \frac{R_i + R_j}{2} \tag{6}$$

where $r_\mu \in]0, 1]$ is a dimensionless radius. R_i and R_j are respectively the radius of particles i and j in contact. The internal cohesive forces between two particles i and j are given by the following system:

$$\begin{bmatrix} F_n^{j\to i} \\ F_t^{j\to i} \\ M^{j\to i} \end{bmatrix} = \begin{bmatrix} \frac{E_\mu A_\mu}{L_\mu} & 0 & 0 & 0 \\ 0 & \frac{12E_\mu I_\mu}{L_\mu^3} & \frac{6E_\mu I_\mu}{L_\mu^2} & \frac{6E_\mu I_\mu}{L_\mu^2} \\ 0 & \frac{6E_\mu I_\mu}{L_\mu^2} & \frac{4E_\mu I_\mu}{L_\mu} & \frac{2E_\mu I_\mu}{L_\mu} \end{bmatrix} \begin{bmatrix} u_n^i - u_n^j \\ u_t^i - u_t^j \\ \theta_i \\ \theta_j \end{bmatrix} \tag{7}$$

where θ_i and θ_j are respectively the rotations of particles i and j. $u_n^{i,j}$ and $u_t^{i,j}$ are respectively the normal and tangential displacements. The linear system of equations shows the micro-macro relations applied to determine the contact forces between two particles i and j. These relations stem from the classical stiffness matrix of the beam element model. The translational and rotational equations of motion for a particle i are written as follows:

$$m_i \ddot{u}_i = F_i^{ext} + \sum_j F^{j\to i} \tag{8}$$

$$I_i \ddot{\theta}_i = M_i^{ext} + \sum_j M^{j\to i} \tag{9}$$

where m_i is the elementary mass of the particle i and I_i is the quadratic moment of inertia of the particle i. $F^{j\to i}$ et $M^{j\to i}$ are respectively the force and the moment of interaction of the particle j on the particle i. F_i^{ext} et M_i^{ext} are respectively the external force and moment acting on particle i. The numerical resolution is based on an explicit time integration with a formulation based on a Verlet scheme.

Thermoelastic properties

The present section is dedicated to the description of methodologies leading to the assessment of thermoelastic properties, namely the Effective Thermal Conductivity (ETC), the Effective Young's Modulus (EYM) and the Effective Shear Modulus (ESM). For validation purposes, a homogeneous medium with known properties is considered and effective thermoelastic properties are evaluated and finally compared to the expected values. From now on, the continuous domain is a square and flat plate of side L=3.5 cm and the corresponding ECD is a granular packing composed of about 5000 polydisperse cylindrical particles.

ETC

The ETC is estimated by the following approach. A temperature difference (ΔT) is imposed between two opposite edges of the square domain (in the present case $y = 0$ and y =L). The heat transfer within the homogeneous medium is described by the time-dependent methodology described in subsection a). The heat flux density (ϕ) is then numerically estimated at stationary state and the ETC λ deduced from the following Equation :

$$\lambda = \frac{\phi \mathrm{L}}{\Delta T} \tag{10}$$

In the present test, the plate is subjected to thermal and initial conditions defined as follows :

$$\begin{cases} T_1 : T(y=0) = 25°C \\ T_2 : T(y=\mathrm{L}) = 100°C \\ t=0 : T(y) = T_0 = 25°C \quad 0 < y < \mathrm{L} \end{cases} \tag{11}$$

Lateral boundaries are under adiabatic conditions and material parameters are listed in Tab. 1 :

Table 1. Thermal properties of the continuous domain

Density	ρ_c	2600	kg/m^3
Thermal conductivity	λ	30	W/mK
Specific heat	c_p	900	J/kgK

The variation of temperatures obtained by an analytic solution [10] and the DEM-based approach at times 3 s, 30 s and 150 s are graphically shown in Fig. 4a. Both models present identical temperature profiles which exhibits the ability of the DEM-based approach to model heat transfer in a continuous domain.

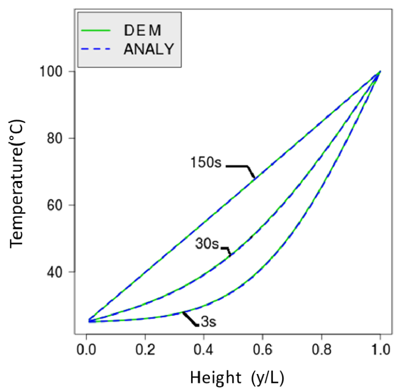

Figure 4. Comparison between analytic and discrete model solutions at several times (a) and field of heat flux density (b)

The heat flux density is estimated at stationary state at the scale of the particle using the following Equation which is analogous to the Love-Weber formulation.

$$\phi_i = \frac{1}{V_i} \sum_j \Phi^{ext,j} x_{ij} \tag{12}$$

where ϕ_i is the heat flux density related to the particle i, V_i is the volume of the particle i, x_{ij} is the length of the contact between particles i and j, and $\Phi^{ext,j}$ is the external flux applied to the particle i by the particle j. The heat flux density ϕ is estimated after averaging heat flux densities over the volume of the plate. In the present example, a value of 64303 W/m^2 is obtained which leads to an ETC λ=30.008 W/(m.K) which is very close to the expected value of 30 W/(m.K). This highlights the ability of the present DEM-based approach to estimate ETC of homogeneous materials.

EYM and ESM

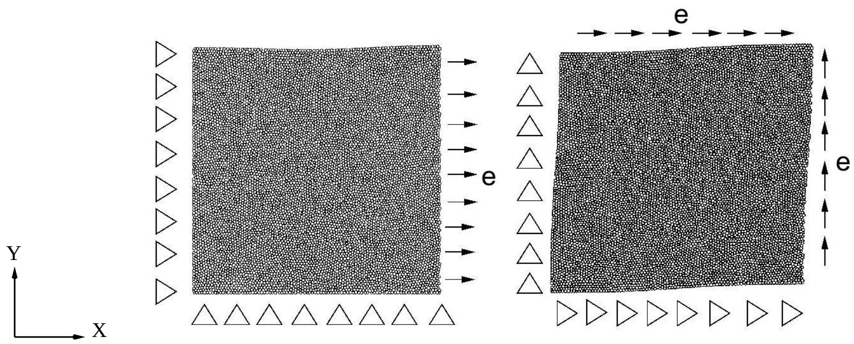

Figure 5. Quasi-static tensile (a) and shear (b) tests

EYM and ESM are estimated via quasi-static tensile and shear tests performed under a plane stress state using the boundary conditions described in Fig. 5. Symmetry boundary conditions are considered and a displacement e is imposed on the right edge of the square in the case of the tensile test on the one hand, on the other hand anti-symmetry boundary conditions are considered and a displacement e is imposed on top and right edges of the plate in the case of the shear test. The main issue of such an approach is that on the contrary of FE calculations for which local properties at the scale of the element are identical to the macroscopic properties in the case of a homogeneous material, microscopic properties of the beam element (E_μ, r_μ) can only be correlated to EYM and ESM as previously done in previous works [7, 8].

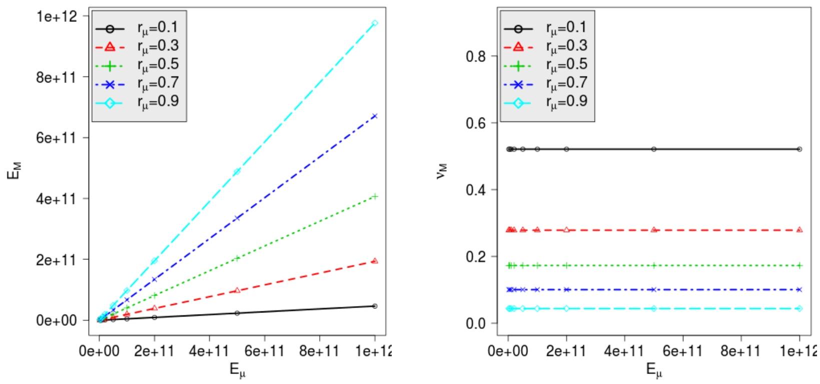

Figure 6. Influence of the microscopic parameters E_μ and r_μ on the EYM (a) and the Poisson's ratio (b)

The calibration process consists in determining the relation between microscopic and macroscopic parameters via a full range of investigated configurations so that the evolution of microscopic properties allows us to choose the desired macroscopic ones. In the present work, we consider a microscopic Young's modulus in the interval [2GPa, 1000GPa], and a r_μ parameter in the interval $[0.1, 0.9]$. Evolution curves are plotted in Figures 6-a and -b. We notice that the macroscopic Poisson's ratio ν_M does not depend on E_μ but quadractically depends on the dimensionless radius r_μ. EYM E_M linearly depends on r_μ and quadratically depends on E_μ. These conclusions are in good agreement with those obtained by André et al. [7] in the context of spheres in 3D.

Case of a heterogeneous continuous medium with a single inclusion

The section is dedicated to the investigation of the thermoelastic behavior of a heterogeneous continuous medium with a single inclusion. For this purpose a 2D square-shaped representative pattern of the composite material is generated and numerical approaches described in the previous section are considered. The representative pattern consists of a centred circular inclusion which represents the unidirectional fibre and has a radius equal to 0.25 times the length L (Fig. 7). The square pattern is discretized by the same random granular packing constituted of 5000 polydisperse particles than the previous one used for a homogeneous material.

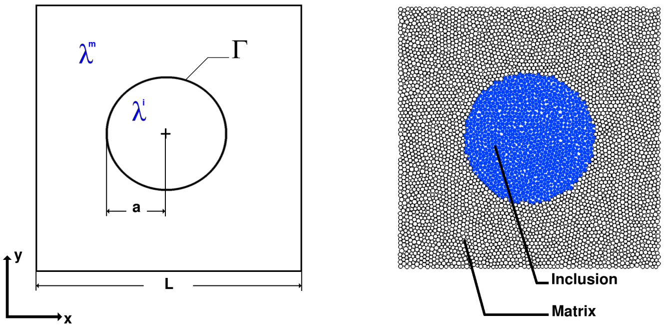

Figure 7. Single inclusion problem: continuous (a) and discrete (b) models

Thermal properties

Our objective is to assess the ETC λ^e of the heterogeneous continuous medium with a single inclusion via the proposed DEM-based approach. Both inclusion and matrix phases are supposed isotropic with thermal conductivities respectively denoted by λ^i and λ^m where superscripts i and m designate the inclusion and matrix phase respectively. λ^m is set to 30 W/(m.K) and λ^i is varied according to the expected contrast of properties $c_\lambda = \frac{\lambda^i}{\lambda^m}$ which can be chosen greater or lower than 1. In other words, the inclusion can be considered more conductive or more insulative than the matrix phase. The specific heat capacity is supposed set to 900 J/(K.kg) for both phases but this is of little importance since we are only interested by results at stationary state in the present section. The evaluation of the ETC is performed considering the methodology described in subsection a). Results are compared to two numerical homogenization techniques. The first technique is the FFT-based method which consists in solving the Lippmann-Schwinger's equation in Fourier space using an iterative algorithm [11, 12]. In the present work, calculations are performed using the Eyre-Milton scheme and a digitized map of the representative pattern consisted of 1048576 (1024^2) pixels [13]. The second one is the double-scale homogenization method (2SFEM) [14]. This approach is based on variational considerations and uses the FEM with periodic boundary conditions. Results are also compared with the classical FEM for which thermal conditions are the same as those considered in the DEM-based approach, and a theoretical estimate, namely the Hashin's model (HM) [15]. For information purposes, all FEM calculations are carried out using a structured mesh composed of 980000 (2×700^2) 3-node triangular elements.

Table 2. Influence of the contrast on the normalized ETC for several numerical and theoretical approaches

c_λ		0.01	0.02	0.05	0.1	0.2	0.5	1	2	5	10	20	50	100
λ^*	DEM	0.672	0.678	0.694	0.722	0.768	0.877	1.000	1.139	1.300	1.382	1.432	1.466	1.478
	FEM	0.677	0.682	0.698	0.723	0.769	0.878	1.000	1.140	1.302	1.384	1.433	1.467	1.478
	2SFEM	0.676	0.682	0.698	0.723	0.768	0.877	1.000	1.140	1.301	1.383	1.433	1.466	1.477
	FFT	0.677	0.682	0.698	0.723	0.768	0.877	1.000	1.140	1.302	1.384	1.433	1.467	1.472
	HM	0.677	0.683	0.698	0.723	0.769	0.877	1.000	1.140	1.301	1.383	1.432	1.465	1.477

Calculations are carried out for a range of c_λ from 0.01 to 100. Thus, two main configurations are considered, namely the case of an inclusion more insulative than the matrix ($c_\lambda < 1$) and the reverse case for which the inclusion is more conductive than the matrix ($c_\lambda > 1$). Table 2 illustrates the influence of the contrast on the assessed normalized ETC (λ^*) which is obtained by dividing the ETC λ^e by the thermal conductivity of the matrix. Results are compared with those obtained using other numerical and theoretical approaches. Whatever the contrast, less or more than 1, predictions given by the DEM are very close to other assessments with a maximum relative difference of 0.6%. This highlights the ability of the DEM to estimate the ETC of a heterogeneous continuous medium with a single inclusion.

Elastic properties

Tensile and shear tests are carried out using the boundary conditions already seen in Fig. 5 in order to assess EYM and ESM. The macroscopic Young's modulus E^m of the matrix is set to 65 GPa. Different values of macroscopic Young's modulus E^i of the inclusion are considered so that the contrast of properties $c_r = \frac{E^i}{E^m}$ varied from 0.01 to 100. Poisson's ratios of both phases are set to 0.3 and we suppose a plane stress state. DEM-based results are compared to those obtained using the same numerical approaches than previously seen for evaluating the ETC, namely the FFT-based method, the double-scale homogenization method (2SFEM), the classical FEM for which boundary conditions are identical to those considered in the DEM approach. Comparisons are also performed with the theoretical estimate given by Mori and Tanaka (MT) [16]. For information purposes, all FE and FFT-based calculations are carried out considering the same discretizations than previously used for evaluating the ETC.

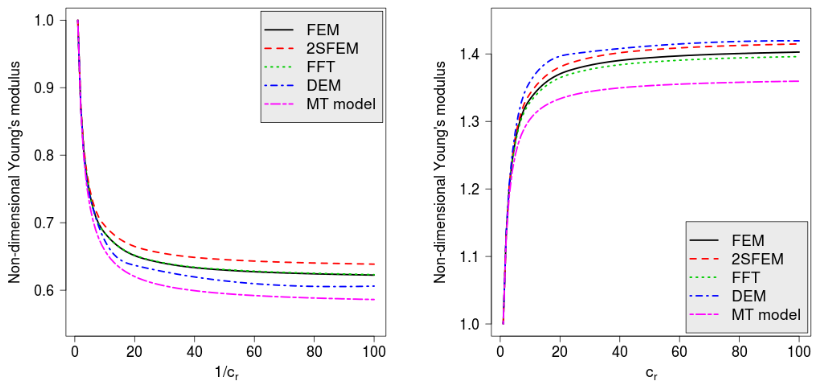

Figure 8. Non-dimensional Young's modulus as a function of the contrast of properties, case $c_r \leq 1$ (a) case $c_r \geq 1$ (b)

Two configurations are investigated. The first problem corresponds to the case of an inclusion less stiff than the matrix with a Young's modulus less than that of the matrix. The second one corresponds to the case of an inclusion stiffer than the matrix with a Young's modulus higher than that of the matrix. Fig. 8 illustrates the influence of the contrast of properties c_r on the non-dimensional Young's modulus which is obtained by dividing E by E^m. Results exhibit a good agreement between DEM, FEM, numerical homogenization techniques and the theoretical estimate whatever c_r. For example, for a contrast of 100, the relative differences with respect to the value given by the FEM is 5.39% for the Young's moduli in the case where $c_r < 1$, and the relative difference is only 0.06% when $c_r > 1$. Globally, relative differences do not exceed 5% whatever the considered contrast of properties. This highlights the ability of the DEM approach to estimate elastic properties of a heterogeneous continuous medium with a single inclusion.

Conclusion

The present paper dealt with a DEM-based approach for characterizing the thermoelastic behavior of composite materials. A focus was done on a 2D plate structure with a single inclusion embedded in a matrix. Comparisons with other numerical and theoretical approaches highlight the suitability of the proposed approach to estimate ETC, EYM and ESM. These results are encouraging and pave the way to interesting prospects. In a next future, we expect to extend the present approach to model the thermomechanical behavior of complex heterogeneous media where fracture phenomena and interfacial effects arise.

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