ANALYSIS OF HETEROGENEOUS MICROSTRUCTURES BY THE BOUNDARY ELEMENT METHOD CONSIDERING PLASTICITY

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Abstract. *A formulation of the Boundary Element Method (BEM) to perform elasto-plastic analysis of heterogeneous microstructures is presented. Inside the matrix can be defined voids or inclusions with different elastic properties and governed by different constitutive models. The microstructure is modelled by a zoned plate, where different values of Poisson's ratio and Young's modulus can be defined for each sub-region. To solve the domain integrals written in terms of in-plane displacements or plastic forces, the matrix and inclusions domains have to be discretized into cells where the displacements and forces are approximated. In the microstructure or RVE (representative volume element) the displacement field is defined as a sum of a linear part plus the displacement fluctuation, being its non-linear problem solved in terms of displacement fluctuations. Adopting homogenization techniques, the homogenized values for stress and constitutive tensor can be computed after solving the RVE equilibrium problem. Some numerical examples are presented whose results are compared to a finite element code to show the model accuracy.*

Keywords: *Boundary elements, Zoned plates, Plasticity, Multi-scale analysis, Homogenization techniques.*

1 INTRODUCTION

The boundary element method (BEM) has already proved to be a suitable numerical tool to deal with plate problems. The method is particularly recommended to evaluate internal force concentrations due to loads distributed over small regions that very often appear in practical problems. Several works have already considered BEM formulations to treat different kinds of problems as can be seen in the works Aliabadi (2002), Beskos (1991), Brebbia et al. (1984), Fernandes & Souza Neto (2013) and Fernandes & Rosa Neto (2015).

In general, the materials, even the metallic, are heterogeneous at the micro and grain scale. Besides, the material microstructure can be also appropriately manipulated by adding certain constituents to a matrix phase, in order to change the material properties to attend specific applications, as the MMCs (metal matrix composites). As any heterogeneity of the material as well as the microcracking initiation and propagation in the micro-scale affect directly the macro-continuum response, modelling heterogeneous material in different scales is very important to better represent the behaviour of such complex materials as discussed in Gal & Kryvoruk (2011), Nguyen et al (2011) and Nemat-Nasser & Hori (1999).

In the multi-scale analysis considered in this work, the RVE (representative volume element) represents the microstructure, at grain level, of the macro-continuum at the infinitesimal material neighborhood of a point as can be seen in the works Souza Neto & Feijóo (2006) and Fernandes et al (2015 a, b). In this paper a BEM formulation to perform elasto-plastic analysis of RVEs is developed, where it is considered as a zoned plate, whose sub-regions define the different materials of the microstructure.

2 BASIC EQUATIONS

The domain Ω of a heterogeneous microstructure is assumed to consist in general of a solid part, Ω^s and a void part Ω^v, being $\Omega = \Omega^v \cup \Omega^s$, where the solid part can be made of distinct materials (or phases), each one defined by a sub-domain, whose material can have different elastics properties. Without loss of generality, let us consider the microstructure depicted in Fig. 1 represented by a zoned plate, where sub-region $\boldsymbol{\Omega_1}$ represents the matrix whose external boundary is Γ_1, sub-region $\boldsymbol{\Omega_2}$ is an inclusion and $\boldsymbol{\Omega_3}$ a void. Besides, in Fig. (1) Γ_{jk} represents the interface between the adjacent sub-regions $\boldsymbol{\Omega_j}$ and $\boldsymbol{\Omega_k}$ and the Cartesian system of co-ordinates (axes x_1 and x_2) is defined on the plate surface.

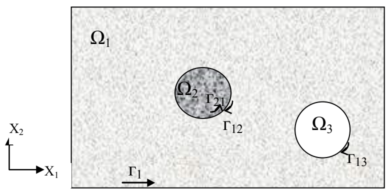

Figure 1- Heterogeneous microstructure represented by a zoned plate

For a point placed at any of those sub-regions, the in-plane equilibrium equation can be defined:

$$\dot{N}_{ij},_j + \dot{b}_i = 0 \qquad \text{i, j=1, 2} \tag{1}$$

where b_i are body forces distributed over the plate middle surface and N_{ij} is the membrane internal force.

As this work only deals with small strain problems the total strain will be split into its elastic and inelastic parts, $\dot{\varepsilon}_{ij}^{e}$ and $\dot{\varepsilon}_{ij}^{p}$ respectively, as follows:

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{p} \qquad \text{i, j= 1, 2} \tag{2}$$

By applying the Hooke's law the stress tensor rate $\dot{\sigma}_{ij}$ (as well as the force $\dot{N}_{ij}$) is related to the elastic part $\dot{\varepsilon}_{ij}^{e}$ of the strain tensor rate and the membrane force predictor $\dot{N}_{ij}^{e}$ (often defined as elastic trial used in non-linear algorithms) related to the total strain $\dot{\varepsilon}_{ij}$. Thus, the forces $\dot{N}_{ij}^{e}$, for plane stress conditions, can be written in terms of the in-plane deformations ε_{ij} as follows:

$$\dot{N}_{ij}^{e} = \frac{\overline{E}}{\left(1-\nu^2\right)}\left[\nu\, \dot{\varepsilon}_{kk}\delta_{ij} + \left(1-\nu\right)\dot{\varepsilon}_{ij}\right] \tag{3}$$

where $\overline{E} = Et$, E is the Young's modulus, ν the Poisson's ratio, t the plate thickness and δ_{ij} the Kronecker delta. Therefore, the inelastic membrane force rate $\dot{N}_{ij}^{p}$ is defined as:

$$\dot{N}_{ij}^{p} = \dot{N}_{ij}^{e} - \dot{N}_{ij} \tag{4}$$

Observe that although an elastic-plastic criterion has been adopted in the present work for describing the dissipative process in the RVE, the presented BEM formulation used to model the macro-continuum can be also used with other kind of criteria. The problem definition is then completed by assuming the following boundary conditions over Γ: $U_i = \overline{U}_i$ on Γ_u (in-plane displacements) and $P_i = \overline{P}_i$ on Γ_p (in-plane tractions), where $\Gamma_u \cup \Gamma_p = \Gamma$.

3 INTEGRAL REPRESENTATION FOR DISPLACEMENT

As developed in Fernandes & Rosa Neto (2015), from Betti's Theorem, the following equation can be obtained for any sub-region Ω_m:

$$\int_{\Omega_m} \varepsilon_{kij}^{m*} N_{ij}^{m} d\Omega = \int_{\Omega_m} N_{kij}^{m*} \varepsilon_{ij}^{m} d\Omega - \int_{\Omega_m} \varepsilon_{kij}^{m*} N_{ij}^{p(m)} d\Omega \qquad \text{i, j, k=1, 2} \tag{5}$$

where ε_{kij}^{m*} and N_{kij}^{m*} are fundamental solutions.

Equation (5) can be now modified by writing the fundamental strains of sub-region Ω_m in terms of the values ε_{kij}^{*} and $\overline{E}$ referred to the sub-region where the load point s is placed. This simplifies the formulation because allows to eliminate the tractions along the interfaces. Thus, as developed in Fernandes & Rosa Neto (2015), the following relation can be defined:

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$$\varepsilon_{kij}^{m*} = \varepsilon_{kij}^{*}\overline{E} / \overline{E}_m \tag{6}$$

where $\overline{E}_m = E_m t_m$, being E_m the Young's modulus in the sub-region Ω_m.

Considering Eq. (3) the membrane force N_{kij}^{m*} can be also written in terms of ν and N_{kij}^{*} referred to the sub-region where the load point is placed as follows:

$$N_{kij}^{*(m)} = \frac{\left(1-\nu^2\right)\nu_m}{\left(1-\nu_m^2\right)\nu} N_{kij}^{*} + \frac{\overline{E}}{\left(1-\nu_m^2\right)}\left(1-\frac{\nu_m}{\nu}\right)\varepsilon_{kij}^{*} \tag{7}$$

Replacing Eqs. (6) and (7) into (5) and considering all sub-regions, one obtains the following relation for the whole plate:

$$\int_{\Omega} \varepsilon_{kij}^{*} N_{ij} d\Omega = \sum_{m=1}^{N_S}\left[\frac{\overline{\overline{E}}_m}{\overline{\overline{E}}}\frac{\nu_m}{\nu}\int_{\Omega_m}\varepsilon_{ij}N_{kij}^{*}d\Omega + \overline{\overline{E}}_m\left(1-\frac{\nu_m}{\nu}\right)\int_{\Omega_m}\varepsilon_{ij}\varepsilon_{kij}^{*}d\Omega_m\right] - \int_{\Omega_m}\varepsilon_{kij}^{*}N_{ij}^{p(m)}d\Omega \quad \text{i, j, k=1, 2} \tag{8}$$

where N_s is the sub-regions number; $\overline{\overline{E}}_m = \dfrac{\overline{E}_m}{\left(1-\nu_m{}^2\right)}$

Integrating Eq. (8) by parts we obtain the following representation of in-plane displacements:

$$\begin{aligned}
C_{k1}\dot{u}_1(s) + C_{k2}\dot{u}_2(s) = &-\frac{\overline{\overline{E}}_1\nu_1}{\overline{\overline{E}}\nu}\int_{\Gamma_1}\left(\dot{u}_1(P)p_{k1}^{*}(s,P) + \dot{u}_2(P)p_{k2}^{*}(s,P)\right)d\Gamma + \\
&-\sum_{m=1}^{N_{inc}}\frac{\left(\overline{\overline{E}}_m\nu_m - \overline{\overline{E}}_1\nu_1\right)}{\overline{\overline{E}}\nu}\int_{\Gamma_{m1}}\left(\dot{u}_1(P)p_{k1}^{*}(s,P) + \dot{u}_2(P)p_{k2}^{*}(s,P)\right)d\Gamma_{m1} \\
&-\sum_{m=1}^{N_{voids}}\frac{\overline{\overline{E}}_1\nu_1}{\overline{\overline{E}}\nu}\int_{\Gamma_{1m}}\left(\dot{u}_1(P)p_{k1}^{*}(s,P) + \dot{u}_2(P)p_{k2}^{*}(s,P)\right)d\Gamma_{1m} + \int_{\Gamma_1}\left(u_{k1}^{*}(s,P)\dot{p}_1(P) + u_{k2}^{*}(s,P)\dot{p}_2(P)\right)d\Gamma + \\
&-\overline{\overline{E}}_1\left(1-\frac{\nu_1}{\nu}\right)\int_{\Gamma_1}\left[\dot{u}_1(P)\varepsilon_{k1}^{*}(s,P) + \dot{u}_2(P)\varepsilon_{k2}^{*}(s,P)\right]d\Gamma + \sum_{m=1}^{N_s}\overline{\overline{E}}_m\left(1-\frac{\nu_m}{\nu}\right)\int_{\Omega_m}\dot{u}_i(p)\varepsilon_{kij,j}^{*}(s,p)d\Omega_m \\
&-\sum_{m=1}^{N_{inc}}\left[\overline{\overline{E}}_m\left(1-\frac{\nu_m}{\nu}\right) - \overline{\overline{E}}_1\left(1-\frac{\nu_1}{\nu}\right)\right]\int_{\Gamma_{m1}}\left[\dot{u}_1(P)\varepsilon_{k1}^{*}(s,P) + \dot{u}_2(P)\varepsilon_{k2}^{*}(s,P)\right]d\Gamma_{m1} + \int_{\Omega_m}\varepsilon_{kij}^{*}\dot{N}_{ij}^{p(m)}d\Omega \quad \text{k, i,j=1,2}
\end{aligned} \tag{9}$$

where k is the fundamental load direction, N_{int} is the interfaces number; N_{voids} is the voids number; Ω_1 represents the matrix domain and Γ_1 its external boundary; Γ_{m1} represents an interface between the matrix and inclusion m and Γ_{1m} the interface between the matrix and a void m; the free terms values C_{k1} and C_{k2} depend on the position of the collocation point s.

4 ALGEBRAIC EQUATIONS

The integral representation Eq. (9) is transformed into algebraic expression after discretizing the external boundary and interfaces into elements and the domain into cells. Geometrically linear elements have been adopted, where linear shape functions have been assumed to approximate the variables. Moreover, triangular cells have been used to discretize the sub-regions domain, where the displacements u_1 and u_2 are approximated by continuous linear shape functions, being their cell nodal values new independent values. Besides, the plastic forces are assumed to be constant over the cell domain.

Along the external boundary the nodal values are: two in-plane displacements (u_1 *and* u_2) and two in-plane tractions (p_1 and p_2). As two of these values must be given as boundary conditions, two equations must be written for each boundary node. Besides, two displacement (u_1 *and* u_2) are also defined at interface and cell nodes and three plastic forces (N_{11}^{p}, N_{12}^{p} and N_{22}^{p}) are defined at cells nodes. Therefore two more displacements integral equations are required at interfaces and cells nodes and three elastic forces equations have to be written at cells nodes. After writing all required equations, one can get the following set of equations where all values are written in terms of theirs increments:

$$\begin{bmatrix} [H]_{BB} & [H]_{Bi} \\ [H]_{iB} & [H]_{ii} \end{bmatrix} \begin{Bmatrix} \{\Delta U\}_B \\ \{\Delta U\}_i \end{Bmatrix} = \begin{bmatrix} [G]_{BB} \\ [G]_{iB} \end{bmatrix} \{\Delta P\}_B + [E]\{\Delta N^p\} \tag{10}$$

In Eq. (10) the subscript B is related to the external boundary while i is referred to interface and internal nodes; $\{\Delta N^p\}$, $\{\Delta U\}$ and $\{\Delta P\}$ are plastic forces, displacement and traction incremental vectors, respectively; $[H]$ is obtained by integrating all boundary and interfaces elements as well as the cells defined in the matrix and inclusions domain; $[G]$ is computed by integrating all boundary elements and [E] obtained after integrating all cells.

In a multi-scale analysis, the macro-strain has to be imposed to the RVE, leading to prescribe linear displacements over the external boundary as boundary conditions. Thus, in this case the unknowns vector $\{\Delta X\}$ computed from Eq. (10) is given by:

$$\{\Delta X\} = \begin{Bmatrix} \{\Delta P\}_B \\ \{\Delta U\}_i \end{Bmatrix} = \{\Delta L\} + [R]\{\Delta N^0\} \tag{11}$$

where $\{\Delta L\}$ gives the elastic solution and [R] represents the effect of the plasticity over the RVE.

To solve the RVE equilibrium problem we also need to write the elastic forces at all cell nodes, which is given by the following algebraic equation:

$$\{\Delta N^e\} = -[[H']_c \quad [H']_i] \begin{Bmatrix} \{\Delta U\}_c \\ \{\Delta U\}_i \end{Bmatrix} + [G']_c \{\Delta P\}_c + [E']\{\Delta N^0\} \tag{12}$$

After imposing the boundary conditions, Eq. (12) can be written as:

$$\{\Delta N^e\} = \{\Delta K_N\} + [S]\{\Delta N^0\} \tag{13}$$

where $\{\Delta K_N\}$ gives the elastic solution and [S] represents the effect of the plasticity over the RVE.

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5 HOMOGENISED VALUES FOR STRESS AND CONSTITUTIVE TENSOR

In the multi-scale analysis, the stress as well as the constitutive tensor at a point x of the macro-continuum is evaluated from their respective fields over the RVE by using homogenization techniques. For that, the RVE is assumed sufficiently large in order to be considered as a continuum and the concept of stress to be valid at the microscopic scale. Then, it is also assumed that the strain tensor ε and the stress tensor σ at a point x of the macro-continuum are the volume average of their respective microscopic field (ε_μ or σ_μ) over the RVE associated with x (see Souza Neto & Feijóo (2006), Fernandes et al (2015 a,b)), i. e.:

$$\varepsilon(x) = \frac{1}{V_\mu} \int_{\Omega_\mu} \varepsilon_\mu(y) dV \tag{14}$$

$$\sigma(x) = \frac{1}{V_\mu} \int_{\Omega_\mu} \sigma_\mu(y) dV \tag{15}$$

where ε and σ are, respectively, the macroscopic or homogenised strain and stress.

The homogenised constitutive tangent modulus C^{ep} can be also evaluated by applying the homogenization process, as follows:

$$C^{ep}(x) = \frac{\partial \sigma(x)}{\partial \varepsilon(x)} = \frac{\frac{1}{V_\mu} \int_{\Omega_{\mu S}} \partial \sigma_\mu(y) dV}{\partial \varepsilon(x)} = \frac{\frac{1}{V_\mu} \int_{\Omega_{\mu S}} \partial f_y(\varepsilon_\mu(y)) dV}{\partial \varepsilon(x)} \tag{16}$$

Note that in a non-linear analysis f_y would be the constitutive functional defined by the adopted criterion. As in this work no dissipative phenomenon is considered, f_y is given by the elastic tensor.

The final expressions for homogenised stress and constitutive tensor are obtained according to the formulation proposed in Souza Neto & Feijóo (2006). For that, let us now split the microscopic displacement field u_μ in the following sum:

$$u_\mu(y) = u_\mu^L(y) + \tilde{u}_\mu(y) \tag{17}$$

In Eq. (17) $u_\mu^L(y)$ represents a linear displacement field, being $u_\mu^L(y) = \varepsilon(x) y$, where $\varepsilon(x)$ is the macroscopic strain and y represents the coordinates of an arbitrary point of the RVE; $\tilde{u}_\mu$ is the displacement fluctuation which represents the strain variation in the RVE.

After discretising the RVE into cells and elements (or finite elements for the FEM formulation developed in the works Souza Neto & Feijóo (2006), Fernandes et al (2015 a,b), the following microscopic equilibrium equation must hold for a discretisation h:

$$R_h = \int_{\Omega_\mu^h} B^T f_y(\varepsilon + B\tilde{u}_\mu) dV = \sum_{e=1}^{N_{cel}} B_e^T N^e A_e = 0 \tag{18}$$

where Ω_μ^h denotes the discretised RVE domain, N_{cel} is the number of cells used to discretize the RVE, B_e the cell strain-displacement matrix, A_e is the cell area and N^e the normal force vector in the cell, which is considered constant over the cell.

After imposing the macroscopic strain tensor ε to the RVE boundary, the microscopic equilibrium problem consists of finding the displacement fluctuation field $\tilde{u}_\mu^{i+1} = \tilde{u}_\mu^i + \delta\tilde{u}_\mu^{i+1}$ that satisfies Eq. (18), being $\delta\tilde{u}_\mu^{i+1}$ the fluctuations corrections to be imposed in iteration *i+1*. Thus, by applying the Newton-Raphson Method, $\delta\tilde{u}_\mu^{i+1}$ is computed by the following expression:

$$F^i + K^i \delta\tilde{u}_\mu^{i+1} = 0 \tag{19}$$

where F is the traction vector and K the rigidity matrix, being defined as:

$$F^i = \int_{\Omega_\mu^h} B^T f_y\left(\varepsilon_{n+1} + B\tilde{u}_\mu^i\right) dV = \sum_{e=1}^{N_{cel}} B_e^T N^{e(i)} A_e \tag{20}$$

$$K^i = -\frac{\partial R_F}{\partial \tilde{u}} = \sum_{e=1}^{N_{cel}} B_e^T D_N^e B_e A_e \tag{21}$$

where D_N is the microscopic constitutive tangent relating forces and strains.

The RVE formulation is completed with the choice of kinematical constraints to be imposed on the RVE that leads to different classes of multi-scale models and therefore, to different numerical results. Three different boundary conditions can be imposed to the RVE in terms of displacement fluctuations: (i) linear boundary displacements, (ii) periodic fluctuations and (iii) uniform tractions (see more details in Souza Neto & Feijóo (2006), Fernandes et al (2015 a,b)). According to the formulation developed in Souza Neto & Feijóo (2006), the homogenised stress tensor (eq. 15) can be written as:

$$\sigma = \frac{1}{2V_\mu}\left(\bar{\sigma} + \bar{\sigma}^T\right) \tag{22}$$

where $\bar{\sigma} = \sum_{i=1}^{Nb} \{F_b\}_i \{y\}_i^T$, being N_b the number of external boundary nodes and the forces F_b are obtained from the forces P_b defined in Eq. (11), multiplying P_b by the influence length of the respective node.

It is important to point out that the forces P_b defined in Eq. (11) are computed considering the nodal displacements along the external boundary U_b obtained after solving the RVE equilibrium problem, i. e., U_b is given by adding the displacement fluctuation field $\tilde{u}$ to the linear displacement field u^L.

As discussed in Souza Neto & Feijóo (2006), the homogenised constitutive tangent modulus C^{ep} (Eq. 16) can be split into two parts, as follows:

$$C^{ep} = C^{ep(Taylor)} + \tilde{C}^{ep} \tag{23}$$

where $C^{ep(Taylor)}$ is denoted the Taylor model tangent operator (obtained by assuming $\nabla^S \tilde{u}_\mu = 0$) and computed by the volume average of the microscopic constitutive tangent; $\tilde{C}^{ep}$ represents the influence of the displacement fluctuation into the homogenised tangent modulus; they are given by (Souza Neto & Feijóo (2006)):

$$C^{ep(Taylor)} = \frac{1}{V_\mu} \int_{\Omega_\mu} \frac{\partial \sigma_\mu}{\partial \varepsilon_\mu} dV = \frac{1}{V_\mu} \int_{\Omega_\mu} D_\mu dV = \sum_{p=1}^{N_p} \frac{V_p}{V_\mu} D_\mu^p \tag{24}$$

$$\tilde{C}^{ep} = \frac{\frac{1}{V_\mu} \int_{\Omega_\mu^h} \partial g_y \left(\nabla^S \tilde{u}_\mu\right) dV}{\partial \varepsilon} = -\frac{1}{V_\mu} G_R K_R^{-1} G_R^T \tag{25}$$

where D_μ is the microscopic constitutive tangent and N_p the number of phases defined in the RVE; $G = \sum_{e=1}^{Ncel} D_\mu^e B_e V_e$; K_R and G_R are, respectively, reduced forms of K (Eq. 21) and G, being they defined according to the adopted multi-scale model (see Souza Neto & Feijóo (2006), Fernandes et al (2015 a,b)).

6 NUMERICAL APPLICATION

In the numerical example is considered the RVE depicted in Fig. 2, where five voids are defined. For the matrix the following material properties are adopted: Poisson's ratio ν*=0,3;* Young's modulus *E=200GPa*, yield stress σ_y*=200MPa* where a plastic Von Mises model with isotropic hardening *K=30GPa* has been assumed. In the discretization (see Fig. 2) 546 cells and 357 nodes have been defined in the RVE. Note that in order to show the robustness of the proposed modelling, the voids distribution adopted for the RVE is random and it has been chosen in order to introduce strong heterogeneities due to different sizes and locations of the voids. The macro strain imposed to the RVE boundary is given by: $\{\varepsilon\} = \{\varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_{12}\} = \{-0{,}00045 \quad 0{,}0015 \quad 0\}$.

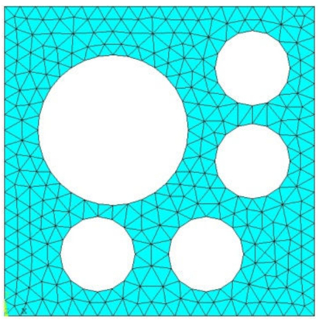

Figure 2- Discretization of a RVE with voids.

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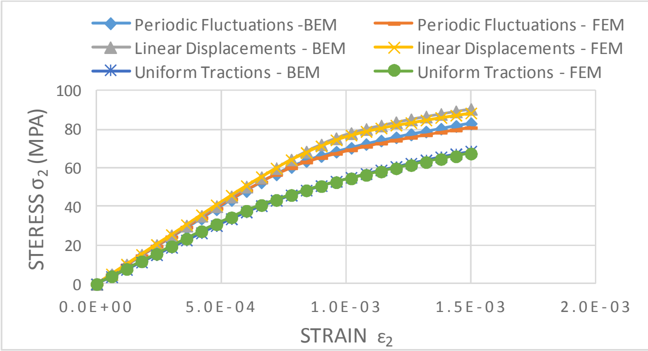

Figure 3- Stress σ2 for different boundary conditions

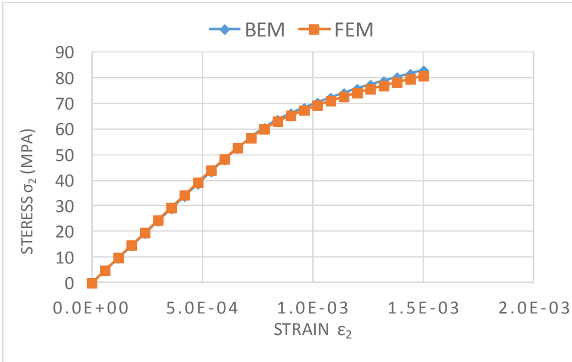

Figure 4- Stress σ2 for periodic fluctuations

In Fig. 3 is presented the stress σ_2 for three different boundary conditions in terms of displacements fluctuations: (i) linear boundary displacements, (ii) periodic fluctuations and (iii) uniform tractions. As expected, linear displacements give the stiffest solution, while uniform tractions the more compliant solution. In Fig. 4, the stress σ_2 for periodic fluctuations are compared to the one obtained with the RVE formulation developed in Fernandes et al (2015 a,b) using the Finite Element Method and in Table 1 is shown the homogeneized constitutive tensor for this case and strain ε_2.=0,0015. As can be observed, the results are very similar.

Table 1: Homogenized Constitutive Tensor considering periodic fluctuations

BEM	FEM
$\begin{bmatrix} 70,144 & 14,395 & -0,9657 \\ 14,395 & 24,606 & -0,7690 \\ -0,9657 & -0,7690 & 13,300 \end{bmatrix}$	$\begin{bmatrix} 69,158 & 14,841 & -1,1215 \\ 14,841 & 25,055 & -0,5560 \\ -1,1215 & -0,5560 & 14,365 \end{bmatrix}$

7 CONCLUSIONS

A BEM formulation to analyze micro-structures of heterogeneous materials has been presented, where the RVE (Representative Volume Element) is modeled as a zoned plate. The different phases of the RVE can have either elastic or elasto-plastic behavior, where different material properties can be defined in order to represent the material heterogeneity. The homogenized values for stress and constitutive tensor have compared very well to the FEM solution, showing the accuracy of the presented formulation.

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