A BOUNDARY ELEMENT BASED MESO-ANALYSIS ON THE EVOLUTION OF MATERIAL DAMAGE

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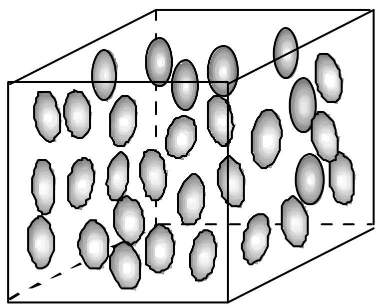
ABSTRACT

In this paper, we present efficient numerical formulations for the analyses of particulate composites, underging meso-structural changes such as particle fracture, stress induced phase transformation, etc. The formulations are derived based on the homogenization method and the boundary element method (BEM). Proposed formulations can efficiently deal with problems, in which particles randomly distribute and orient in the composites, by combining analytical solutions for the ellipsoidal inclusions such as Eshelby's tensor and the boundary element method. Hence, there is no need to carry out any numerical integrations for the particles. Proposed numerical methods are computationally efficient and accurate. The formulations and numerical results for effective elastic moduli of composites and problems of particle fracture and stress induced phase transformation, are presented.

INTRODUCTION

In this paper, efficient boundary element formulations (see [1-6] for the boundary element method) for solids containing ellipsoidal inclusions/particles, as shown in Fig. 1, are presented (see Ashby [7] for various types of composite materials). First, a boundary element based formulation for homogenization analysis is discussed and is combined with analytical solutions for ellipsoidal inclusions in which constant initial strains are specified inside of them. A special case of the analytical solutions is given as the well known Eshelby's tensor [8,9]. The analytical solutions for ellipsoidal inclusions such as Eshelby's tensor, are based on the fundamental solution of linear isotropic elasticity, which is also used in the boundary element method as its kernel functions. The analytic solutions and boundary element formulation can easily be combined.

Homogenization method [10-12] based on the finite element method has been applied to a various class of problems, such as identifying macroscopic elastic moduli and nonlinear behavior of meso-structure for a prescribed macroscopic deformation mode. Homogenization method assumes that the microstructure of solid is spatially periodic, and finite element analyses for a unit of periodic structure (unit cell) are carried out. However, the homogenization method can not be applied to the problems of particulate composite materials in a straight forward manner, since the orientations and distributions of particles



Densely Distribute Particles

Figure 1: Particulate composite material

would be somewhat random. Therefore, defining a unit cell model containing one or a few particles may be an over simplification of the problem. To accurately model such solids, a unit cell containing many particles should be analyzed. Thus, one needs to build and carry out analyses for a unit cell model having tens and hundreds of particles. Finite element model, which is required for such analyses, would be gigantic. Generating the finite element model as well as solving the problem would pose many problems. However, mechanical interactions between the particles, and between matrix material and particles are fully accounted for, when the finite element method is adopted.

On the other hand, methodologies in micromechanics, such as self-consistent method [9,13,14] and Mori-Tanaka theory [9,15] have been presented. For particulate composites, Eshelby's tensor [8,9], takes a central role (see, for example, [9,16,17]). These methodologies have advantages over the finite element method such that the effective mechanical behaviors of composites can be estimated in a closed or semi-closed form, based on the elastic moduli of matrix and particles, the distribution, orientation and volume fraction of the particles. Large scale computations are not required. However the methods in micromechanics do not account for detailed mechanical interactions between the distributed particles. The mechanical interactions may have significant roles when the particles are densely distributed or when we attempt to account for the damage evolution or meso-structural changes, such as phase transformation of the particles.

Boundary element based homogenization formulation, which is developed in this paper, have advantages of both the above mentioned methodologies. Since the method is based on the boundary element method (BEM [1-6]), detailed mechanical interactions between all the material constituents can be accounted for. This nature is similar to that of the finite element method. A unit cell modeled by the boundary element method can contain many particles and the computation is simplified by using analytical solutions for ellipsoidal inclusions, such as Eshelby's tensor [8,9]. In this regard, proposed method is similar to the methodologies in micromechanics.

HOMOGENIZATION FORMULATION FOR PARTICULATE COMPOSITES

In this section, equation formulations for boundary element based homogenization analysis for particulate composites are briefly discussed (see [18,19] for homogenization method based on BEM). In homogenization method, the microstructure of solid is assumed to be spatially periodic, as shown in Fig. 2. A unit of the periodic microstructure is modeled by the boundary element method and is called "unit cell". As shown in Fig.1 in a two dimensional illustration, the size of the unit cell is represented by ε. We introduce two different coordinate systems. One is x_i coordinate system, which is fixed in space and the other is y_i coordinate system, which is scaled by the size ε of unit cell, as:

$$y_i = x_i/\varepsilon + c_i \qquad (1)$$

where c_i are the components of an arbitrary vector. Displacements u_i are expressed by the two scale asymptotic expansion, by following Guedes and Kikuchi [10], as:

$$u_i(\boldsymbol{x},\boldsymbol{y}) = u_i^o(\boldsymbol{x},\boldsymbol{y}) + \varepsilon u_i^1(\boldsymbol{x},\boldsymbol{y}) + \varepsilon^2 u_i^2(\boldsymbol{x},\boldsymbol{y}) + \varepsilon^3 u_i^3(\boldsymbol{x},\boldsymbol{y}) + \cdots \qquad (2)$$

For small deformation linear elasticity problem, Hooke's law and the equation of linear momentum balance are written to be:

$$\sigma_{ij} = E_{ijk\ell}\frac{\partial u_k}{\partial x_\ell} \quad , \quad \frac{\partial \sigma_{ij}}{\partial x_i} + b_j = 0 \qquad (3)$$

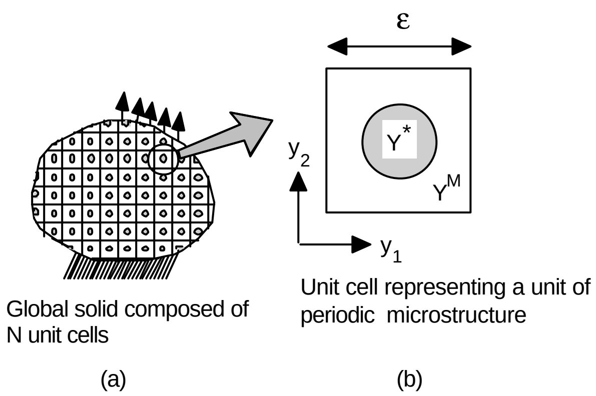


Figure 2: Two dimensional illustration for a solid whose microstructure is periodic and its unit cell.

where $E_{ijk\ell}$ are the fourth order tensor, representing Hooke's law. Based on Eqns. (2) and (3), it can be shown that $u_i^o = u_i^o(x)$ [u_i^o are the functions of x_i only.], and one can obtain an integral equation formulation for u_i^1 for the analysis of unit cell (see Okada et al. [19] for the derivation).

$$C_{pq}u_q^1\left(x_m^Y\right) = \int_{\partial Y} t_j^Y u_{jp}^*\left(y, x_m^Y\right) d(\partial Y) - \int_{\partial Y} t_{kp}^*\left(y, x_m^Y\right) u_k^1 d(\partial Y) - \int_{Y^*} E_{ijk\ell}^M \bar{e}_{k\ell} \frac{\partial u_{ip}^*\left(y, x_m^Y\right)}{\partial y_j} dY^* - \frac{\partial u_k^o}{\partial x_m}\left[\int_{\partial Y} t_{kp}^*\left(y, x_m^Y\right) y_m d(\partial Y) + C_{pq}x_q^Y\right] \tag{4}$$

where $\bar{e}_{k\ell}$ are the fictitious initial strains, which are defined by,

$$\bar{e}_{ij} = C_{ijmn}^M \left(E_{mnk\ell}^* - E_{mnk\ell}^M\right)\left\{\frac{\partial u_k^o(x)}{\partial x_\ell} + \frac{\partial u_k^1(x,y)}{\partial y_\ell}\right\} \tag{5}$$

Displacements u_i^1 at the source point x_m^Y is evaluated by the integral equation (4). A two phase composite material is assumed and elastic constants for matrix and second phase materials are represented by $E_{ijk\ell}^M$ and $E_{ijk\ell}^*$, respectively. u_{ip}^* and t_{ip}^* are the Kelvin solutions (see [4]). Y and ∂Y represent the domain and boundary of the unit cell. Y^* denotes the region of second phase material in Y.

We assume that the solid contains ellipsoidal particles as its second phase material and that the stresses and strains are constant values inside a particle, by following the result of Eshelby [8] and many of micromechanics analyses [9,17]. We then rewrite the volume integral term of integral equation (4), as:

$$\int_{Y^*} \frac{\partial u_{ip}^*\left(y, x_m^Y\right)}{\partial y_j} E_{ijk\ell}^M \bar{e}_{k\ell} dY^* = \sum_{I=1}^{N} \bar{e}_{ij}^I \int_{(Y^*)^I} \frac{\partial u_{ip}^*\left(y, x_m^Y\right)}{\partial y_j} E_{ijk\ell}^M d\left(Y^*\right)^I = \sum_{I=1}^{N} \Lambda_{pij}^I\left(x_m^Y\right) \bar{e}_{ij}^I \tag{6}$$

where $\Lambda_{pij}^I\left(x_m^Y\right)$ are the analytical expressions for the integral (see Mura[9]) and $\bar{e}_{k\ell}^I$ are the fictitious initial strain in the Ith particle. Thus, we write:

$$C_{pq}u_q^1\left(x_m^Y\right) = \int_{\partial Y} t_j^Y u_{jp}^*\left(y, x_m^Y\right) d(\partial Y) - \int_{\partial Y} t_{kp}^*\left(y, x_m^Y\right) u_k^1 d(\partial Y) - \sum_{I=1}^{N} \Lambda_{pij}^I\left(x_m^Y\right) \bar{e}_{ij}^I - \frac{\partial u_k^o(x)}{\partial x_m}\left[\int_{\partial Y} t_{kp}^*\left(y, x_m^Y\right) y_m d(\partial Y) + C_{pq}x_q^Y\right] \tag{7}$$

When the source point x_i^Y is at the interior of the Jth particle, we can derive an integral equation for the displacement gradients $\partial \hat{u}_i / \partial y_j$, by differentiating Eqn. (7) with respect to x_i^Y, as:

$$\left(\frac{\partial \hat{u}_p}{\partial y_q}\right)^J = \int_{\partial Y} t_j^Y \frac{\partial u_{jp}^*\left(y, x_m^Y\right)}{\partial x_q} d(\partial Y) - \int_{\partial Y} \frac{\partial t_{kp}^*\left(y, x_m^Y\right)}{\partial x_q} \hat{u}_k d(\partial Y) - \sum_{\substack{I=1 \\ I \neq j}}^{N} \Theta_{pqij}^I\left(x_m^Y\right) \bar{e}_{ij}^I - S_{pqk\ell}^J \bar{e}_{k\ell}^J \tag{8}$$

where $S_{pqk\ell}^J$ are the components of Eshelby's tensor [8,9] for the Jth particle. Singular volume integrals, whose numerical evaluations are known to be troublesome, are replaced by the analytical formulae such as Eshelby's tensor. Therefore, proposed integral equations are computationally efficient and accurate.

Taking the last term in Eqn. (7) as the forcing term and following the standard boundary element analysis procedures by imposing the so called periodic boundary conditions on displacements u_i^1 and tractions t_i^Y, we can evaluate the displacements and tractions at the boundary of the unit cell. An initial strain iteration method is adopted to obtain the equilibrium (see [5,6] for the initial strain iteration for solving elastic-plastic problems using BEM). Thus, the solutions for given $\partial u_i^o / \partial x_j$ are obtained. We repeat the analyses for six times for a three dimensional problem to determine the responses of microstructure to all the macroscopic deformation modes (six strain modes). The characteristic functions $F_{ik\ell}(y)$, which relate $\partial u_i^o / \partial x_j$ to u_i^1, and the effective elastic moduli $E_{ijk\ell}^H$ of the composite are written to be:

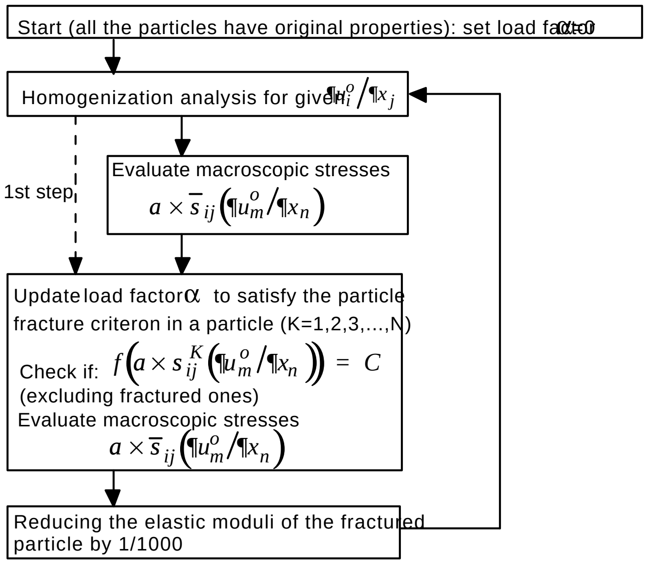


Figure 3: Algorithms for the analysis of problem of particle fracture

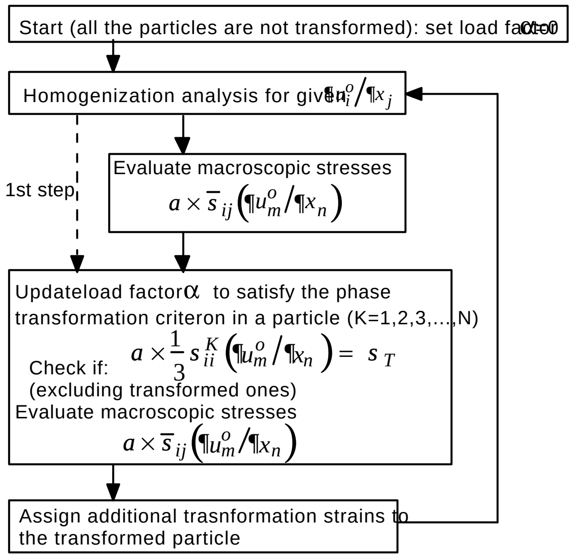


Figure 4: Algorithms for the analysis of problem of stress induced phase transformation

$$\begin{cases} E^H_{ijk\ell}(\boldsymbol{x}) = E^M_{ijk\ell} + \dfrac{1}{|Y|}\sum_{I=1}^{N}\left(E^*_{ijk\ell} - E^M_{ijk\ell}\right)Y_I^* + \dfrac{1}{|Y|}\sum_{I=1}^{N}\left(E^*_{ijk\ell} - E^M_{ijk\ell}\right)\left(\dfrac{\partial F_{mk\ell}(\boldsymbol{y})}{\partial y_n}\right)_I Y_I^* \\ u_i^1 = F_{ik\ell}(y)\dfrac{\partial u_k^o}{\partial x_\ell} \end{cases} \tag{10}$$

ANALYSIS FOR PROGRESSIVE DAMAGE (MESO-STRACTURAL CHANGE)

Here, we deal with the problems of particle fracture and of the stress induced phase transformation of particles (see [17,20] for stress induced phase transformation). We make small extensions on the integral equations (7) and (8), as follows.

Particle Fracture

An incremental analysis is carried out for the problems of particle fracture. The simplest scenario is assumed that when the stresses in a particle satisfy a criterion for particle fracture, the elastic modulus of the particle reduces to zero (in actual calculation, the elastic modulus is reduced to be 1/1000 of the original value). Therefore, the analysis is entirely based on the elastic analysis for the unit cell. The integral equations, which are developed in the previous section, are applied by specifying different elastic moduli for fractured and unfractured particles. Algorithms for the analysis are shown in Fig. 3.

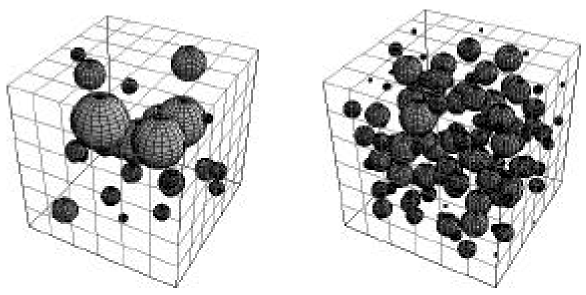
Stress Induced Phase Transformation of Particles

The problems of dilatational stress induced phase transformation (see Okada et al. [17]) are considered and an incremental algorithm is adopted. It is assumed that at the instance, when hydrostatic stress ($\sigma_{kk}/3$) inside a particle reaches a critical value, the particle transforms its phase and dilatational transformation strain is produced. The dilatational transformation strain is modeled as an additional initial strain. The integral equations [Eqns. (7) and (8)] are modified to include the effects of the transformation strain, as:

$$C_{pq}u^1_q\left(x^Y_m\right) = \int_{\partial Y} t^Y_j u^*_{jp}\left(y, x^Y_m\right)d(\partial Y) - \int_{\partial Y} t^*_{kp}\left(y, x^Y_m\right)u^1_k d(\partial Y) - \sum_{I=1}^{N}\Lambda^I_{pij}\left(x^Y_m\right)\bar{\varepsilon}^I_{ij} + \sum_{I=1}^{N}\beta^I\Lambda^I_{pij}\left(x^Y_m\right)\bar{\bar{\varepsilon}}^I_{ij} - \frac{\partial u^o_k(x)}{\partial x_m}\left[\int_{\partial Y} t^*_{kp}\left(y, x^Y_m\right)y_m d(\partial Y) + C_{pq}x^Y_q\right] \tag{11}$$

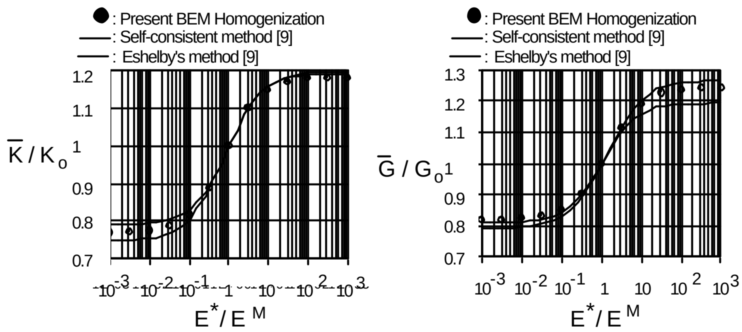
$$\left(\frac{\partial \hat{u}_p}{\partial y_q}\right)^J = \int_{\partial Y} t^Y_j \frac{\partial u^*_{jp}\left(y, x^Y_m\right)}{\partial x_q}d(\partial Y) - \int_{\partial Y}\frac{\partial t^*_{kp}\left(y, x^Y_m\right)}{\partial x_q}\hat{u}_k d(\partial Y) - \sum_{\substack{I=1\\ I\neq j}}^{N}\Theta^I_{pqij}\left(x^Y_m\right)\bar{\varepsilon}^I_{ij} - S^J_{pqk\ell}\bar{\varepsilon}^J_{ik\ell} + \sum_{\substack{I=1\\ I\neq j}}^{N}\beta^I\Theta^I_{pqij}\left(x^Y_m\right)\bar{\bar{\varepsilon}}^I_{ij} + \beta^J S^J_{pqk\ell}\bar{\bar{\varepsilon}}^J_{ik\ell} \tag{12}$$

where $\bar{\bar{\varepsilon}}^I_{ij}$ are fictitious initial strains, which are related to the dilatational transformation strain ε^t, as:



(a) (b)

Figure 5: Distributions of spherical particles in the unit cell. (a) 27 particles whose volume fraction is 0.1, (b) 125 particles whose volume fraction is 0.089



(a) (b)

Figure 6: The results for effective elastic moduli (125 particles). (a) Bulk modulus, (b) Shear modulus.

$$\bar{\bar{\varepsilon}}^{I}_{ij} = C^{M}_{ijk\ell} E^{*}_{k\ell mm}\left(\frac{1}{3}\varepsilon^{t}\right) \tag{13}$$

The effective stress for the solid can be given as average values of stresses in the unit cell, as:

$$\bar{\sigma}_{ij} = E^{M}_{ijk\ell}\frac{\partial u^{o}_{k}}{\partial x_{\ell}} + \frac{1}{|Y|}\sum_{I=1}^{N}\left(E^{*}_{ijk\ell} - E^{M}_{ijk\ell}\right)\left(\frac{\partial \hat{u}_{k}}{\partial \ell}\right)^{I} - \sum_{I=1}^{N}\beta^{I} E^{*}_{ijkk}\left(\frac{1}{3}\varepsilon^{pt}\right) \tag{14}$$

Algorithms for the analysis of the stress induced phase transformation problem are given in Fig. 4.

RESULTS OF NUMERICAL ANALYSIS

A limited number of numerical results are presented in this section due to the restriction of pages (results for the problem of particle fracture are omitted.). Unit cell models used for numerical computations are shown in Fig. 5. Randomly distributed spherical particles are assumed. The volume fraction of the particles is about 10%, and the number of the particles are 27 and 125. Linear quadrilateral boundary elements are used. Total number of boundary elements on each face of the unit cell is 36 (6 x 6).

Evaluation for Effective Elastic Moduli

The results are shown in Fig. 6. Isotropic elasticity is assumed for the particles and the ratio of Young's moduli of matrix and particles are varied from 10^{-3} to 10^{3}. Poisson's ratio is assumed to be 0.3 for both the material constituents. Results, which are analyzed by the 125 particle model, are presented.

For a comparison purpose, the results obtained by using self-consistent method and Eshelby's method theory (see Mura [9]) are also plotted in the figures. The results by three different methods are within an agreement. Though exact solutions are not known, three different methods are within a reasonable agreement and, therefore, the proposed technique is, at least, proven to be reliable.

Stress Induced Dilatational Transformation

Relationships between the effective hydrostatic stress ($\bar{\sigma}_{kk}/3$) and effective dilatational strain ($\partial u^{o}_{i}/\partial x_{i}$), when Young's moduli of matrix and of particles are set to be the same, are shown in Fig. 7. Dilatational transformation strain is assumed to be $\varepsilon^{t}_{kk} = 0.05$ and the phase transformation is assumed to take place when the hydrostatic stress in a particle reaches transformation stress σ_{T}. The elastic moduli for matrix and particles are set to be the same in this case.

The stress-strain relationships follow zigzag paths and have negative slopes while the phase transformation is undergoing. The path is smoother for the 125 particle model than for the 27 particle one.

CONCLUDING REMARKS

In this paper, a new but simple method for the analysis of particulate composite material is presented. Though the numerical results, which are presented here, are rather limited, the method is proven to be quite effective. If one carried out a three dimensional analysis with 125 randomly distributed particles in a unit cell using the finite element method, a large scale computation must be carried out and the state of art mesh generation software would be necessary for the generation of analysis model. All the numerical analyses, which are presented in this paper are carried out using a workstation within a reasonable amount of computational time. Therefore, it can be concluded that present numerical technique can deal with the meso-mechanics problems of particulate composites effectively and efficiently.

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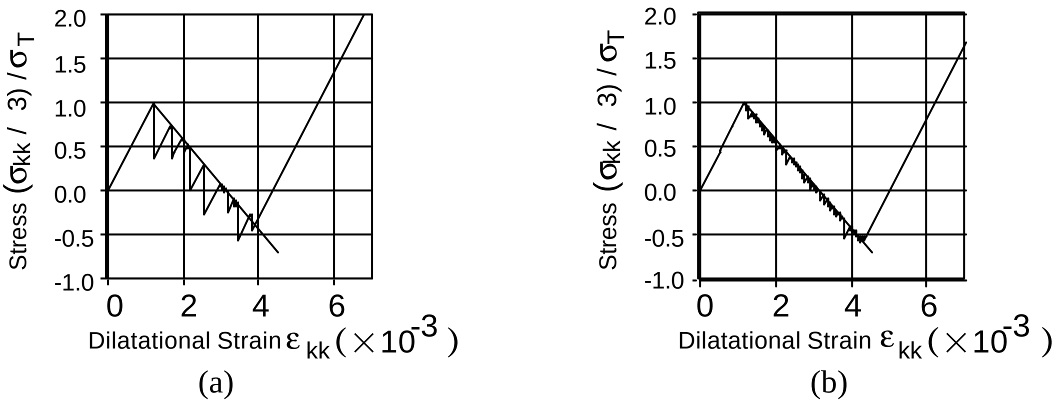

Figure 7: Hydrostatic pressure stress-dilatational strain curves for the problems of stress induced phase transformation. (a) 27 spherical particles, (b) 125 spherical particles. The straight lines are stress-strain curves following the results of Ramakrishnan, Okada and Atluri [20].