Boundary Element Analysis of Heat Transfer in Anisotropic Functionally Graded Materials

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Summary

A Boundary Element Method (BEM) for analysis of plane steady-state heat transfer problems in generally anisotropic solids which are in perfect or imperfect contact is developed. Thermal conductivities in each solid are considered to be constant or exponentially graded in a fixed but arbitrary direction. Contact conditions are applied in weak form, which permits an easy coupling of non-conforming meshes at contact zones. Numerical results presented demonstrate the applicability of the computational code developed for the analysis of thermal barrier coatings fabricated with isotropic or anisotropic Functionally Graded Materials (FGM).

Introduction

FGM represent a new generation of composites with spatial variation of composition and consequently also of materials properties. They are used in many areas [1] and in particular in high-temperature turbine engines as thermal barrier coatings of metallic turbine blades made out of single-crystal superalloys. The advantage of FGM thermal barrier coatings is that they release stresses by gradually changing the properties through their thickness in such a way that they are similar to the metallic substrate at their interface and similar to the pure ceramic at the external surface. The anisotropic nature of the single crystal blade subjected to a thermo-elastic loading may have a substantial influence in the heat flux and the stresses generated within the blade.

Computational analysis of FGM, in particular in design optimisation and assessment of crack initiation and propagation, is of major importance for their development and applications, due to the fact that their manufacturing and experimental testing are complex. For the analysis required by FGM the Boundary Element Method (BEM) [2] has significant advantages versus the Finite Element Method (FEM) [3] due to its inherent feature of providing accurate results in analysis of problems with presence of cracks, interface cracks, notches, corners and contact zones. All this makes BEM particularly suitable for the study of failure in FGM thermal barrier coatings.

A general 2D BEM code for a numerical analysis of steady-state heat transfer in solids composed by several materials in a perfect (with zero resistance to heat flow) or imperfect (with some finite resistance to heat flow) contact has been developed. Contact

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conditions are imposed using a weak formulation [4,5], which is very advantageous when using non-conforming meshes with non-matching nodes at contact zones. Note that non-conforming meshes are useful in case of: a) strongly non-conforming contact surfaces, b) application of adaptive methods on some subdomains, c) independently generated meshes, d) coupling of BEM meshes with boundary elements of different kind. Materials analysed by the present BEM code can be isotropic or anisotropic and homogeneous or exponentially graded in any fixed direction. Fundamental solutions (and their derivatives) for these materials applied in the code have been developed in [6,7,8].

As an example of the possible applications of the BEM code developed a problem of a homogeneous substrate protected by an FGM thermal barrier coating from a high temperature in presence of a debonding modelled like an interface crack is solved. Two cases, with isotropic and anisotropic materials considered for the substrate and coating, have been solved.

Heat Transfer Problem for FGM

Consider a plane exponentially-graded anisotropic solid D with a piecewise smooth boundary ∂D. Let the thermal conductivities of D be expressed as:

$$k_{ij}(\mathbf{x}) = K_{ij}\exp\{2\boldsymbol{\beta}\bullet\mathbf{x}\} \quad \mathbf{x}=(x_1,x_2)\in D, \quad i,j=1,2, \tag{1}$$

where the constant vector $\boldsymbol{\beta}=(\beta_1,\beta_2)$ represents the direction and magnitude of variation. Vector $\boldsymbol{\beta}$ can be real or pure imaginary. Matrix $\mathbf{K}$ is symmetric and positive definite ($K_{ij}=K\delta_{ij}$ for isotropic materials). The normal heat flux associated to the unit outward normal vector $\mathbf{n}(\mathbf{x})$ at $\mathbf{x}\in\partial D$ is given as $q(\mathbf{x})=-n_i(\mathbf{x})k_{ij}(\mathbf{x})T_{,j}(\mathbf{x})$ where $T(\mathbf{x})$ represents the solid temperature. Then, the Fourier law can be expressed, in terms of temperature, as:

$$-\left(K_{ij}T_{,ij}(\mathbf{x}) + 2\beta_i K_{ij}T_{,j}(\mathbf{x})\right)\exp\{2\boldsymbol{\beta}\bullet\mathbf{x}\} = Q(\mathbf{x}) \tag{2}$$

where $Q(\mathbf{x})$ represents the volumetric heat generation. Let the boundary be partitioned as follows: $\partial D=\partial D_T\cup\partial D_q\cup\partial D_R\cup\partial D_{pc}\cup\partial D_{ic}$, boundary conditions being then defined as: $T=\overline{T}$ in ∂D_T, $q=\overline{q}$ in ∂D_q, $T-T_0=R_T q$ in ∂D_R, where $\overline{T}$ and $\overline{q}$ respectively are the prescribed temperature and normal heat flux, T_0 is the environmental temperature and R_T is the convection resistance which can be a function of the point. Thermal contact conditions between two solids (A and B) are expressed as follows: $q^A+q^B=0$, $T^A-T^B=0$ in ∂D_{pc}; $q^A+q^B=0, T^A-T^B=R_T q^A$ in ∂D_{ic}; where ∂D_{pc} and ∂D_{ic} are respectively the zones of perfect and imperfect thermal contact.

BEM for FGM

The fundamental solution of equation (2) has recently been obtained in [8]:

$$G(\mathbf{x},\mathbf{y}) = -\frac{K_0(.\,R)e^{-\boldsymbol{\beta}\bullet(\mathbf{x}+\mathbf{y})}}{2\pi\sqrt{\det\mathbf{K}}} \tag{3}$$

where $. = \sqrt{\boldsymbol{\beta}\bullet\mathbf{K}\boldsymbol{\beta}}$, $R = \sqrt{\mathbf{r}\bullet\mathbf{K}^{-1}\mathbf{r}}$ with $\mathbf{r} = \mathbf{x}-\mathbf{y}$, and K_0 is the modified Bessel function of the zero order. The normal heat flux, through a plane defined by the unit normal vector $\mathbf{n} = \mathbf{n}(\mathbf{x})$, associated to $G(\mathbf{x},\mathbf{y})$ can be expressed according to [8] as:

$$\frac{.\,G(\mathbf{x},\mathbf{y})}{.\,.\,x} = -n_i(\mathbf{x})K_{im}e^{2\boldsymbol{\beta}\bullet\mathbf{x}}\frac{.\,G(\mathbf{x},\mathbf{y})}{.\,x_m} = -\frac{e^{\boldsymbol{\beta}\bullet\mathbf{r}}}{2\pi\sqrt{\det\mathbf{K}}}\left(\frac{.}{R}(\mathbf{n}\bullet\mathbf{r})K_1(.\,R) + (\mathbf{n}\bullet\mathbf{K}\boldsymbol{\beta})K_0(.\,R)\right) \tag{4}$$

where K_1 is the modified Bessel function of the first order.

The Boundary Integral Equation (BIE) of an FGM solid can be obtained, in terms of $G(\mathbf{x},\mathbf{y})$ and $.\,G(\mathbf{x},\mathbf{y})/.\,.\,x$, in a similar way as for a homogeneous anisotropic solid with constant thermal conductivities, which corresponds to the particular case of $\boldsymbol{\beta}$=0 [6]. In the case with no heat sources within the volume, this BIE writes as:

$$c_K(\mathbf{y})T(\mathbf{y}) + \int_{.D}\left(\frac{.\,G}{.\,.\,x}(\mathbf{x},\mathbf{y})T(\mathbf{x}) - G(\mathbf{x},\mathbf{y})q(\mathbf{x})\right)\mathrm{d}S_x = 0 \tag{5}$$

where $c_K(\mathbf{y}) = 1$ if $\mathbf{y}\,.\,D$, $c_K(\mathbf{y}) = 0.5$ if $\mathbf{y}$ is a smooth point on the boundary $.\,D$, and in the case of a corner point [6]:

$$c_K(\mathbf{y}) = \frac{1}{2} - \frac{1}{2\pi}\operatorname{sgn}\left(\mathbf{n}^{(1)}\,.\,\mathbf{n}^{(2)}\right)\arccos\left(\mathbf{n}_{,K}^{(1)}\bullet\mathbf{K}\mathbf{n}_{,K}^{(2)}\right), \quad \mathbf{n}_{,K}^{(e)} = \frac{\mathbf{n}^{(e)}}{\sqrt{\mathbf{n}^{(e)}\bullet\mathbf{K}\mathbf{n}^{(e)}}} \tag{6}$$

where $\mathbf{n}^{(1)}\,.\,\mathbf{n}^{(2)} = n_1^{(1)}n_2^{(2)} - n_2^{(1)}n_1^{(2)}$ and $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$ are the unit outwards normal vectors to $.\,D$ at $\mathbf{y}$.

BIE (5) is solved by the BEM implemented following the general procedures described in [2] using linear continuous elements. The integrals are computed numerically over the elements not including the collocation point $\mathbf{y}\,.\,.\,D$. A semianalytical approach has been developed for calculation of the integrals over the elements including the collocation point.

Numerical Example

BEM solution of a problem of a homogeneous substrate protected by an FGM coating from a high temperature in presence of a debonding modelled like an interface crack (Fig. 1) is presented. Two cases have been solved: a) an isotropic substrate (with thermal conductivity K=25.51Wm^{-1}K^{-1}) with an isotropic coating (with thermal conductivity varying between that of the substrate and 2.09Wm^{-1}K^{-1}), and b) an anisotropic substrate (with K_{11}=51.02, K_{22}=25.51 and K_{12}=0Wm^{-1}K^{-1}) with an FGM coating (with thermal conductivity varying exponentially between that of the substrate and K_{11}=4.18, K_{22}=2.09 and K_{12}=0Wm^{-1}K^{-1}). Thermal resistances at the top and bottom surfaces respectively are R_T=5x10^{-4}W^{-1}m^{2}K and R_T=10^{-4}W^{-1}m^{2}K for both cases. Although the BEM code developed can model a finite thermal resistance with a spatial variation along the crack, the results presented correspond to an infinite thermal resistance there.

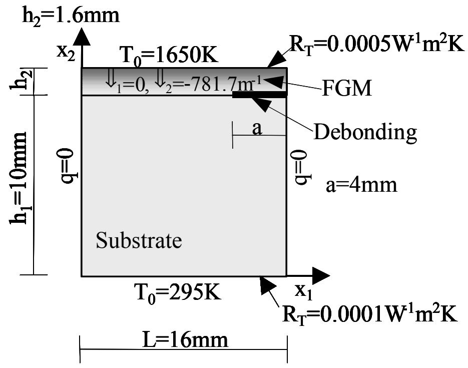

Figure 1: Substrate-FGM coating configuration.

Solutions for T along the lateral surfaces are shown in Fig. 2. At the right-hand side the crack originates a discontinuity in T with a null slope at the crack in accordance with the boundary condition of perfect isolation. Along the left-hand side, far enough from the crack influence, the temperature is approximately linear in the substrate and exponential in the FGM coating and coincident in both cases. This behaviour corresponds to the 1D solution without crack, where the difference in conductivity in the horizontal direction has no influence on the problem solution. Fig. 3 shows the effect of the crack on the temperature variation along the horizontal surfaces. This variation along the crack agrees with the characteristic exponent of the first term of the asymptotic expansion of T at the crack tip, which is equal to 0.5 for both problems (with isotropic and anisotropic materials) [9]. The increments of temperature along the top surface are about 260°C and 170ºC respectively for the isotropic and anisotropic materials, maximum temperature values 1370°C and 1282°C respectively being achieved at points placed above the crack. As could be expected, a decrease in the temperature jump at the interface crack in the anisotropic case (400ºC) in comparison with the isotropic case (580ºC) can be observed.

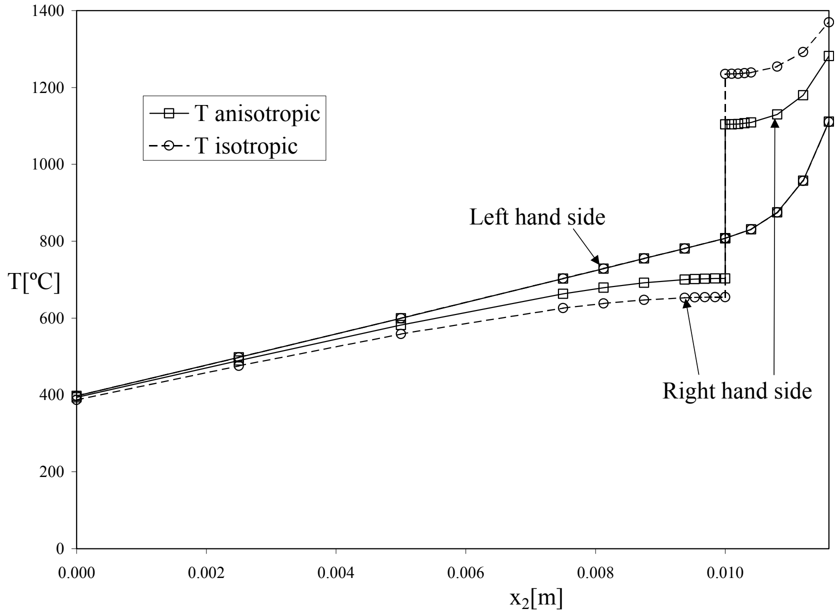

Figure 2. Temperature along lateral surfaces.

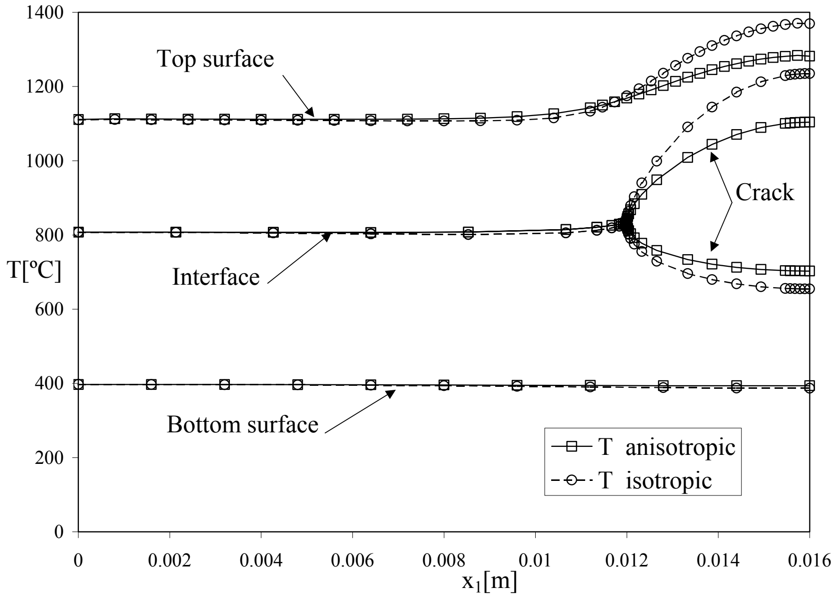

Figure 3. Temperature along horizontal surfaces.

Conclusions

A BEM code for solving plane steady-state heat transfer problems in solids composed by several isotropic and anisotropic materials whose thermal conductivities are constant or exponentially graded in any fixed direction has been developed. Numerical results obtained show that it can be useful in the study of FGM thermal barrier coatings, in particular in presence of defects like debonding, where these defects originate a strong perturbation of the heat flux in their neighbourhood.

Reference

1. Suresh, S. and Mortensen, A. (1998): *Fundamentals of Functionally Graded Materia*ls, Ashgate Publishing.
2. París, F. and Cañas, J. (1997): *Boundary Element Method. Fundamentals and Application*s, Oxford University Press.
3. Lee, Y-D. and Erdogan, F. (1998): "Interface Cracking of FGM Coatings under Steady-State Heat Flow", *Engineering Fracture Mechanics*, Vol. 59, pp 361-380.
4. Blázquez, A., París, F. and Mantič, V. (1998): "BEM Solution of Two-Dimensional Contact Problems by Weak Application of Contact Conditions with Non-Conforming Discretizations", *International Journal of Solids and Structur*es, Vol. 35, pp. 3259-3278.
5. Núñez, J.P., Muñoz, D., Mantič, V. and París, F. (2003): "A Weak Application of Transmission Conditions in 2D BEM with Non-Conforming Meshes for Isotropic and Anisotropic Potential Problems", *Advances in Boundary Element Techniques IV*, R. Gallego and M.H. Aliabadi (Eds.), Queen Mary, University of London, pp. 111-116.
6. Mantič, V. and París, F. (1995): "On Free Terms and Singular Integrals in Isotropic and Anisotropic Potential Theory", *Computational Mechanics 95*, S.N. Atluri, G. Yagawa and T.A. Cruse (Eds.), Springer Verlag, pp. 2806-2811.
7. Gray, L.J., Kaplan, T., Richardson, J.D. and Paulino, G. H. (2002): "Green's Functions and Boundary Integral Equations for Functionally Graded Materials: Heat Conduction", *Journal of Applied Mechanics*, Vol. 70, pp. 543-549.
8. Berger, J.R., Martin, P.A., Mantič, V. and Gray, L.J. (2002): "Fundamental Solutions for Steady-State Heat Transfer in an Exponentially-Graded Anisotropic Material", *Zeitschrift für Angewandte Mathematik und Physik* (in press).
9. Mantič, V., París, F. and Berger, J., (2003): "Singularities in 2D Anisotropic Potential Problems in Multimaterial Corners. Real Variable Approach", *International Journal of Solids and Structur*es, Vol. 40, pp. 5197-5218.