Fracture of functionally graded thermal barrier coating on a homogeneous substrate: models, methods, analysis

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Abstract. Fracture of functionally graded thermal barrier coatings on a homogeneous semi-infinite substrate (FGC/H) is studied under the influence of thermal loadings. A mathematical model for the FGC/H with pre-existing systems of cracks is presented in point of view of the formulation of the boundary conditions and assumptions, and afterwards the integral equations. Methods for solving the problem are described, and then demonstrated for some special cases of the arrangement of cracks. The effect of geometry (the thickness of the coating and location – orientation of multiple cracks) and inhomogeneity parameters of FGs on the main fracture characteristics of the material is analyzed. The study can be used to improve the thermal fracture resistance of FGC/H systems.

1. Introduction
Thermal barrier coatings are widely used in industry, for example, in aerospace and airplane construction, and in power engineering. The effectiveness of rocket equipment, power turbines and aircraft gas turbine engines depends on the operating temperature. High temperatures and abrupt temperature changes lead to high-temperature cracking and melting of metal parts. Thermal barrier coatings create a layer with low thermal conductivity on the surface of the workpiece, which reduces the negative impact of high temperatures. For this purpose, various ceramics are used. Ceramics have a low thermal conductivity, but they are brittle. In addition, as a result of the difference in coefficients of thermal expansion of the coating and the substrate, high thermal stresses at the bond interface occur, which leads to cracking and debonding of the coatings. To overcome this problem, new materials are being sought, and new coatings are designed, namely, layered coatings and coatings from functionally gradient materials [1]. Functionally graded materials (FGMs) are a special class of composites with properties that vary along one direction (one spatial coordinate). Generally, the change in the properties of FGMs is connected with a corresponding variation in the chemical composition and/or physical structure of the material along this direction.

The study of the strength and fracture toughness of such FGMs is of great importance, especially under the combined effect of temperature, mechanical stresses and aggressive environment. Nowadays, a lot of studies has been devoted to these problems, reviews can be found in [1, 2]. However, the interaction of cracks and defects in FGMs under thermal loading is not sufficiently developed.

Investigation of the fracture of the functionally graded coating on a homogeneous substrate (FGC/H) under the influence of thermal loads includes the following tasks:
- Modeling of inhomogeneous physical and mechanical properties of FGMs and the determination of the stress-strain state in FGC/H structures.
- The problem of edge, internal and interface cracks and their interaction.
- The influence of material heterogeneity on the interaction of cracks, as well as the mutual effect of thermal and mechanical loads on cracks and on the interaction of cracks.

In the present paper, the problem of the interaction of systems of cracks (edge and internal) in a functionally graded coating on a homogeneous semi-infinite substrate subjected to thermal loads is considered. The applied methods are similar to those used in reference [3] for an infinite bimaterial formed from functionally gradient and homogeneous materials, and in [4] for a FGM coating on a semi-infinite substrate with a periodic system of edge cracks in the coating.

The paper is organized as follows. The statement of the problem is presented in Section 2, where the geometry of the problem and the loading are described, and also the boundary conditions and assumptions are formulated. Then, in Section 3 models for functionally graded materials (FGMs) and for cracks in FGMs are described. In Section 4 the formulation of integral equations is followed by methods for solving these equations. Afterwards, in Section 5 the main fracture characteristics are calculated, namely, the stress intensity factors, as well as the fracture angles and the critical loads. In Section 6 a few illustrative examples are presented and parametric analysis is performed. Some concluding remarks are made in the final Section 6.

2. Statement of the problem

2.1. Geometry of the problem
The general case of the geometry of the problem is depicted in figure 1a. The upper layer of thickness \( h \) is made from a functionally graded material (FGM), and the semi-infinite substrate consists of a homogeneous material. The functionally graded coating (FGC) and the substrate are perfectly bonded with the exception of an interface crack disposed at the interface between the two materials. The FGC contains arbitrary located cracks of length \( 2a_k \) \((k=1,…,N)\), which can be internal and/or edge cracks. The coordinate systems are chosen as follows: the global coordinates \((x, y)\) with the \( x \)-axis located on the surface of the FGC/H structure and the local coordinates \((x_k, y_k)\) connected with cracks and with centers in the midpoint of the \( k \)-th crack. The crack positions are determined explicitly by the midpoint coordinates \( x_k^0 \) and the inclination angles \( \alpha_k \) to the \( x \)-axis (or \( \beta_k \) for edge cracks, \( \beta_k = -\alpha_k \)) (figure 1b).

2.2. Thermal and mechanical loads
The following loads are considered: a steady state thermal flux applied normal to the surface of the FGC/H structure (figure 1a), a tension parallel to this surface (in the \( x \)-direction), and cooling by \( \Delta T \).

In the case of cooling of the FGC/H structure tensile residual stresses are observed as shown in the experimental investigations [5]. Since the problem is linear, the results for each load can be superimposed. In the case of FGC/H under a heat flux the problem is solved in two steps, first, the thermal problem for the FGC/H structure with cracks, and then the thermo-elastic problem for the same geometry.

2.3. Assumptions
The following assumptions are used for this problem:
- The uncoupled, quasi-static thermo-elasticity theory is applied. In this theory the temperature distribution is independent of the mechanical field, and the solution consists of the determination of the temperature field and then the determination of the thermal stresses.
- The thermal and mechanical properties of an FGC are continuous functions of the thickness coordinate \( y \).
- The non-homogeneity of the functionally graded material is revealed in the form of the corresponding inhomogeneous stress distributions on the surfaces of the cracks [3, 4, 6]. In this case, the properties of the FGM should vary slightly with the depth of the layer.
Figure 1. (a) An FGC/H structure with a system of cracks. (b) Coordinate systems connected with cracks. (c) A partially thermal conducting crack. (d) Partially closed crack with an open zone of length 2c and a system of open or closed cracks.

2.4. Boundary conditions
The thermal problem for a system of thermally insulated cracks in an infinite bimaterial consisting of a functionally graded material and a homogeneous substrate has been formulated in [3]. In the present problem the partially thermal insulated cracks in the FGC are considered with the insulation coefficient $\eta_k$ ($0 \leq \eta_k \leq 1$). The description of the model is given below in Section 3. Cracks are free of stresses, unless other conditions are mentioned. The FGC and the substrate are perfectly bonded, i.e. ideal thermal and mechanical conditions are fulfilled outside an interface crack, namely, the temperatures and the thermal fluxes are equal at the interface, and the stresses and displacements are also equal.

2.5. Methods
For the formulation of the problem the method of complex variables is used, and the method of superposition. Due to the superposition principle the common problem is decomposed into sub-problems, each of which contains one crack. Besides, the loads (thermal and mechanical) at infinity are reduced to the corresponding loads on the crack faces. The solution of each sub-problem can be obtained in explicit form (and can be analyzed separately) or in an integral form, and this integral form is used for constructing the equations of the complete problem. The methods for constructing integral equations for systems of cracks in a homogeneous material can be found in [7].
3. Modeling of functionally graded materials and cracks in FGMs

3.1. Models for functionally graded materials

The thermal and mechanical properties of an FGC are continuous functions of the thickness coordinate \( y \). As in the previous works [3, 8, 9] the exponential form of these properties is used:

\[
f(y) = f_1 \exp(\zeta_n(y + h)), \quad -h \leq y \leq 0
\]

(1)

Here

\[
f = \{k, \alpha_t, E\}, \quad f_1 = \{k_1, \alpha_{t1}, E_1\}, \quad \zeta_n = \{\delta, \varepsilon, \omega\},
\]

\( k \) is thermal conductivity, \( \alpha_t \) – thermal expansion coefficient and \( E \) – the Young’s modulus with non-homogeneity parameters \( \delta, \varepsilon \) and \( \omega \), respectively. \( f_1 \) are thermal and mechanical properties of the homogeneous substrate.

The Poisson’s ratio is assumed to be constant and is equal to the value of the homogeneous substrate. The previous studies show that the effect of Poison’s ratio on the stress intensity factors is negligibly small (see, for example, [10]).

The values of the dimensionless graded parameters \( \zeta_n h \) (\( h \) is the thickness of the FGC) are obtained from Eq. (1) as

\[
\zeta_n h = \ln(f_2 / f_1), \quad f_2 = f(y)|_{y=0}, \quad f_1 = f(y)|_{y=-h}
\]

An example of ceramic/metal FGC/H is \((\text{ZrO}_2/\text{Ti-6Al-4V})/\text{Ti-6Al-4V}\) with \( f_2 / f_1 = \{2/6.7, 10/8.6, 200/114\} \) and, respectively, with the inhomogeneity parameters \( \{\delta h, \varepsilon h, \omega h\} = \{-1.2, 0.15, 0.56\} \) (see [8, 11]). The variation of non-dimensional properties \( f / f_1 = \exp(\zeta_n h(y/h + 1)) \) with dimensionless coordinate \( y/h \) is displayed in figure 2a. The coefficient of thermal expansion and the Young’s modulus increase toward the upper part of the FGC/H structure, while the coefficient of thermal conductivity decreases (figure 2a).

\[\text{Figure 2. The variation of the exponential function } f / f_1 = \exp(\zeta_n h(y/h + 1)) \text{ (a) and the linear function } f(y) = f_1 (1 - \eta_n h(y/h + 1)) \text{ (b) with the coating depth } y/h \text{ for the FGC/H structure.}\]

The exponential form of properties (1) is convenient for the mathematical formulation of equations. Other types of variation laws can be a linear function, a power law or other continuous functions [12]. An example of the linear law for our case is written as

\[
f(y) = f_1 (1 - \eta_n(y + h)) \text{ with } \eta_n = \{\delta, \varepsilon, \omega\}.
\]

(2)
The inhomogeneity parameters are defined as $\eta_h = 1 - f_2 / f_1$, and for the above mentioned ceramic/metal FGC/H structure are the following: $\eta_h = \{ \partial h, \partial h, \partial h \} = \{0.7, -0.16, -0.75\}$. Figure 2b shows the variation of this linear function with coordinate $y/h$.

For practical application, if the spatial composition profile is known, it can be useful to apply a formula based on the rule of mixtures for determining the effective properties of composites. Theoretical mixing laws have been considered extensively for different types of composites, and have been applied to FGMs [13, 14, 15]. For example, the thermal conductivity is defined by

$$k(y) = k_m \left[ 1 + \frac{V_i(y)(k_i - k_m)}{k_m + (k_i - k_m)(1 - V_i(y))/3} \right],$$

where the subscripts $i$ and $m$ stand for the inclusion and matrix properties, respectively. The volume fraction of the inclusion phase $V_i(y)$ is assumed in the form of a power-law function with a non-homogeneity parameter $p$

$$V_i(y) = ((y + h)/h)^p,$$

and the matrix phase is calculated as $V_m = 1 - V_i$.

3.2. Models for cracks

Partially thermally permeable cracks. A model of partially thermally permeable (insulated) cracks is used, figure 1c. The simplest model of partially insulated interfacial crack was used, for example, in [9, 16]. The insulation coefficient $\eta_k (0 \leq \eta_k \leq 1)$ is introduced, here the limiting value $\eta_k = 0$ represents the fully insulating crack and $\eta_k = 1$ – the fully conducting crack. In common case the coefficient $\eta_k(x)$ can be the function of the crack coordinate.

Cracks with contact zones. In the present work possible crack closure and contact of the crack surfaces is taken into account in the model (figure 1d), and its contribution is assessed. Previously, the model of a crack with contact zones was considered in the problem of the interaction between an interface crack and internal cracks in FGM/homogeneous bimaterials under the influence of thermal flux in [17] and under the combination of Mode II load and thermal flux in [18]. It was supposed that the closure of the crack does not affect the temperature distribution, and therefore only the thermoelastic problem was reformulated and solved.

Cracks with plastic zones. The plasticity is considered through a special mode, e.g. Dugdale model [19]. In [20] this model was applied for the problem of the interaction between a system of microcracks and a main crack with plastic zones. This plasticity model allows to formulate the equations within the framework of linear fracture mechanics.

4. Formulation of the integral equations of the problem and solution

4.1. System of singular integral equations

As it was mentioned in Section 2, assuming that the inhomogeneity of the FGM is revealed in the form of the corresponding inhomogeneous stress distributions on the surfaces of cracks, the solution of the boundary value problem of elasticity is reduced to the solution of the system of singular integral equations [3, 6, 7]:

$$\int_{-a_n}^{a_n} \frac{g_n'(t)dt}{t-x} + \sum_{k=1}^{N} \int_{-a_k}^{a_k} [g'_k(t)R_{nk}(t,x) + g_k(t)S_{nk}(t,x)]dt = \pi p_n(x), \quad |x| < a_n,$$

$$n = 1, 2, \ldots, N.$$
Here the unknown functions \( g'_n(x) \) are the derivatives of displacement jumps on the crack lines

\[
g'_{n}(x) = \frac{2\mu}{i(k+1)} \frac{\partial}{\partial x} \left( [u_n] + i[v_n] \right),
\]

where \([u_n]\) and \([v_n]\) are shear and vertical displacement jumps, respectively, on the \(n\)-th crack line, \(\mu = E/(1+\nu)\) is the shear modulus, \(E\) - Young’s modulus, \(\nu\) - Poisson’s ratio, \(k = (3-4\nu)/(1+\nu)\) for the plane strain state and \(k = (3-\nu)/(1+\nu)\) for the plane stress state. In equations (3) an overbar \(\overline{\ldots}\) denotes the complex conjugate.

The regular kernels \(R_{ni}\) and \(S_{ni}\) in equations (3) determine the geometry of the problem, and on the right side of equations (3) the functions \(p_n\) are known functions determined by the load on the crack lines.

For internal cracks, the condition of displacement continuity at crack tips has to be taken into account. The system of equations for the heat conduction problem has a similar form, where the unknowns are the derivatives of temperature jumps on the crack lines, and on the right side of the equations – the known functions of the heat fluxes on the cracks.

### 4.2. Solution of the equations

Many results concerning the interaction of cracks were obtained using methods of integral equations [3, 4, 6-9]. Various numerical methods such as series expansions, boundary element methods and others can be used to obtain an approximate solution. The solutions presented below are obtained for FGM/H structures.

#### 4.2.1. Approximate analytical method.

In the previous works [3, 17, 18] results for an infinite bimaterial consisting of an FGM and a homogeneous material with an interface crack and a system of internal cracks in the FGM were obtained by the small parameter method. The solution of equations (3) was presented in explicit approximate form and was written for the interface crack as

\[
g'_0(x) = g'_00(x) + \lambda^2 g'_10(x),
\]

and the stress intensity factors (SIFs) at the interface crack tips were presented as

\[
k^{\pm}_1 - ik^{\pm}_H = k_0 \left\{ 1 + \lambda^2 \sum_{n=1}^{N} g_n(\alpha_n, \varepsilon_n^n / a_0, \delta_n, \alpha_0) \right\}.
\]

The stress intensity factors are found by the formula [4, 7]

\[
k^{\pm}_n - ik^{\pm}_{nB} = \mp \lim_{x_n \to \pm x_n^a} \sqrt{(a_n^2 - x_n^2)} / a_n g'_n(x_n),
\]

where the upper part of the “\(\pm\)” or “\(\mp\)” signs concerns to the right tip and the lower to the left tip of the crack.

It was assumed that an interface crack is significantly larger in size than internal cracks in the FGM. For this special case the small parameter \(\lambda\) is equal to the ratio of the size of small internal cracks to the interface crack size, i.e. \(\lambda = a / a_0\) with \(a = a_n\). The solution takes into account the interaction of the interface crack and each of the internal cracks (the interaction between small cracks is not accounted). These SIF functions contain parameters of the geometry of the problem (the midpoint coordinates \(z_n^a\) of cracks, the orientation angles \(\alpha_n\) of cracks and the crack sizes) and the parameters of the non-homogeneity of the FGM (\(\delta\) and \(\varepsilon\)). It was shown that the non-homogeneity parameters \(\delta\) and \(\varepsilon\) of thermo-conductivity and of thermal expansion coefficients, correspondingly, notably affect the SIFs of the interface crack. The SIFs can be amplified or shielded by the system of microcracks.
4.2.2. Numerical solution. The solution of the equations is obtained by the method of mechanical quadratures [7, 21]. Applying quadrature formulas based on Chebyshev polynomials, the integral equations (3) reduce to systems of algebraic equations. In [8], a scheme for solving this method is given. After determining the unknowns, the main characteristics of the fracture mechanics are calculated, namely, the stress intensity factors at the crack tips (4) or crack tip opening displacements.

5. Fracture criteria

Experimental and theoretical studies show that with a mixed-mode type of loading, the crack propagation deviates from its original one. In FGMs, a mixed stress-strain state can also arise due to the heterogeneity of the material. Applying a fracture criterion, it is possible to determine the angles of the deflection of the propagation of cracks from their original direction and the critical loads at which this propagation occurs. For example, according to the criterion of maximum normal stresses [22] (the formulation of this criterion and the method of application can be also found in [7]), the crack deflection angle (or the fracture angle) is calculated by the formula

$$\phi_0 = 2 \arctg \left[ k_i - \sqrt{k_i^2 + 8k_{II}^2} \right] / 4k_{II},$$

(5)

where $k_i$ and $k_{II}$ are the stress intensity factors.

The critical stresses are calculated from the expression

$$\cos^3(\phi/2)(k_i - 3k_{II} \tan(\phi/2)) = K_{ICIP} / \sqrt{\pi}.$$

Here $K_{ICIP}$ is the fracture toughness of the material near the crack tip. First, it is obtained the angle of the crack propagation using the results for the calculation of SIFs. Then, the local fracture stability is evaluated. This criterion is the simplest one to employ.

In the minimum strain energy density criterion [23] the strain energy density factor (SDF) is introduced so that it is a quadratic form of SIFs (with coefficients in this form presented as functions of fracture angles). Consequently, it is postulated that the crack will grow in the direction where the SDF is minimal and when this minimum reaches a critical value. This criterion depends on Poisson’s ratio.

The maximum strain energy release rate (SERR) criterion [24] posts that the crack will grow along the direction for which the strain energy release rate reaches a critical value. Note, this critical value is material dependent.

As a result (by using these criteria) the fracture angles are obtained as functions of the geometry of the problem and of the non-homogeneity parameters of the FGC with additional parameters due to thermal loadings. Then, the critical stresses and critical heat fluxes are obtained near cracks (for different crack locations).

In [25], the results for these three criteria were compared for the problem for an infinite FGM/H structure and it was shown that they are nearly the same. In the present work the criterion of maximum normal stresses [22] is applied.

6. Results and analysis

The problem contains geometric parameters, such as the size of the cracks, the coordinates of their centers and the inclination angles, and the thickness of the FGM layer, and the parameters of material inhomogeneity, determined by formulas (1) or (2). The presented model allows analyzing the influence of these parameters on the main characteristics of the problem.

Fig. 3 schematically shows three edge cracks and their deviation angles $\phi$, in Fig. 3a the cracks are of the same size, and in Fig. 3b the length of the first crack is twice the length of the second and third ones. The following parameters were used for the calculation: $h/a = 4$, $d/a = 2$, $a = \max a_k$, $a = 1 \text{mm}$, $\varepsilon_a = -1$ and $\omega_a = 0$. The distance between the cracks is equal to the length of the large crack ($d/a=2$), $\beta = 90^\circ$. At $\varepsilon_a = -1$ the coefficient of thermal expansion increases with the depth of the layer. The
FGC/H structure is cooled by $\Delta T$, in this case tensile residual stresses parallel to the boundary ($y = 0$) arise. With this load, for one edge crack the value of the angle is equal to $\phi = 0^\circ$. The change in the angles $\phi$ due to the interaction of the cracks is shown in Fig. 3. It should be noted that the thermal expansion inhomogeneity coefficient does not greatly affect the deflection angles $\phi$. Earlier it was shown that the coefficient of inhomogeneity of thermal conductivity significantly affects the interaction of cracks [3, 17].

Figure 3. Angles of deflection of the propagation of cracks under thermal loading. (a) Three edge cracks of equal length. (b) Edge cracks of different lengths $a_1=a_2=a_3=0.5a_1$. The distance between the cracks is equal to the length of the large crack $d/a=2$, $\beta = 90^\circ$.

The influence of the remaining parameters, geometrical and physical, will be considered later separately for the corresponding problems for thermal and mechanical loads.

7. Conclusions
A general theoretical formulation of the model for the thermal fracture analysis of functionally graded coatings on a homogeneous substrate (FGC/H) has been performed by means of integral equations. The FGC/H structure with pre-existing systems of interacting cracks in the FGC is subjected to thermal and mechanical loadings. The FGM properties are modeled by continuous functions of the spatial coordinate (the thickness of the coating). This approximate model allows taking into account some special crack models such as the partially thermally permeable cracks and the cracks with contact and plastic zones. The solution of equations is obtained numerically, using the special quadrature formulae for the singular and regular integrals in the integral equations. Besides, an approximate analytical solution previously obtained for a special case, when an interface crack is significantly larger in size than internal cracks in the functionally graded material for an infinite FGM/H structures, is given. In the present study the main emphasis is done on the fracture with multiple crack interactions. At first, the stress intensity factors are calculated, then, using the fracture criterion of maximum normal stresses [22], the crack deflection angles (or the fracture angles) are obtained. An illustrative example is presented to show the influence of the parameters of the problem on the edge crack interaction and their deviation from the initial propagation. Other crack models in the FGC/H structures will be considered in future works. The study of fracture of the FGC/H structures is important for a better understanding of the thermal fracture of graded coatings and for improving the fracture resistance of these systems.

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