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Thermal Fracture of Functionally Graded Coatings with Systems of Cracks: Application of a Model Based on the Rule of Mixtures

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Abstract: This paper is devoted to the problem of the thermal fracture of a functionally graded coating (FGC) on a homogeneous substrate (H), i.e., FGC/H structures. The FGC/H structure was subjected to thermo-mechanical loadings. Systems of interacting cracks were located in the FGC. Typical cracks in such structures include edge cracks, internal cracks, and edge/internal cracks. The material properties and fracture toughness of the FGC were modeled by formulas based on the rule of mixtures. The FGC comprised two constituents, a ceramic on the top and a metal as a homogeneous substrate, with their volume fractions determined by a power law function with the power coefficient λ as the gradation parameter for the FGC. For this study, the method of singular integral equations was used, and the integral equations were solved numerically by the mechanical quadrature method based on the Chebyshev polynomials. Attention was mainly paid to the determination of critical loads and energy release rates for the systems of interacting cracks in the FGCs in order to find ways to increase the fracture resistance of FGC/H structures. As an illustrative example, a system of three edge cracks in the FGC was considered. The crack shielding effect was demonstrated for this system of cracks. Additionally, it was shown that the gradation parameter λ had a great effect on the fracture characteristics. Thus, the proposed model provided a sound basis for the optimization of FGCs in order to improve the fracture resistance of FGC/H structures.



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Keywords: thermal fracture; system of cracks; functionally graded coatings; fracture toughness; rule of mixtures

1. Introduction

Functionally graded coatings (FGCs) are widely used in different engineering structures, e.g., for thermal barrier coatings (TBCs) in gas turbine engine blades and vanes to protect metal components from overheating and melting [1]. Functionally graded materials (FGMs) are a special type of composite, consisting of a graded pattern of material composition and/or microstructures, so that the properties of FGMs vary continuously across spatial coordinates through the depth of the layer. FGCs with a gradual compositional variation from heat-resistant ceramics to fracture-resistant metals have been proposed in order to reduce thermal residual stresses causing delamination and the debonding of interfaces, enhance coating toughness, and improve the long-term performance of TBCs. However, cracks can occur because of initial defects or microcracks that appear during manufacturing or operation. Therefore, the study of the fracture of FGCs is important for a better understanding of the fracture resistance of graded coatings.

At present, great progress has been achieved in the study of the fracture behavior of FGMs and FGM structures. An overview of important trends in the study of the fracture behavior of FGMs is presented in [2], where one can find useful references on a wide range of problems, including the thermal and thermo-mechanical fracture of FGMs and related structures. A recent review [3] includes work on FGM fracture under mechanical loads, especially dynamic and fatigue loads, and discusses crack propagation and crack growth

trajectory in FGMs, as well as the effects of material gradation on crack tip fields and crack growth.

Finite element methods and extended finite element methods are extensively used for the computational modeling of FGMs and cracks in FGMs (see references in [2]). Recently, the methods of peridynamics [4] and the phase field approach [5] have been effectively applied in modeling the complex crack propagation paths in FGMs. In [4], systems of interacting cracks in FGMs, namely a macrocrack and various microcrack configurations, were studied with respect to the shielding effect of microcracks (and improved fracture toughness) or the opposite effect of crack propagation acceleration due to microcracks. In [5], 2D and 3D cracks in FGMs were investigated by the phase field formulation. Finite-discrete element methods are also applied in fracture problems for FGMs. For example, in [6], such a method was used to analyze a coupled thermo-mechanical fracture problem for a system of two interacting edge cracks in an FGM.

Analytical and semi-analytical solutions are important tools in fracture studies for FGMs. They can be used as a separate approach for a study, or as a part of a numerical modeling process. An overview of some of the analytical methods used to solve crack problems in FGMs can be found in [2]. Analytical solutions for steady-state heat transfer in a finite cylinder and a hollow sphere made of an FGM (both undamaged) are presented in [7,8], respectively. For the thermal conductivity coefficient, a power function of two spatial coordinates was used. The Robin boundary condition (also called the third type boundary condition) [9] was adopted for this problem. The choice of this FGM model and these boundary conditions made it possible to derive the exact general analytical solution. The influence of material constants and the conductivity ratio was investigated to shed light on the material selection with respect to the temperature distribution. It should be noted that in [10], the use of the Robin boundary condition in the stationary problem of heat conduction helped to derive explicit representations of the singular terms of the asymptotic expansion of the heat flow in the vicinity of the crack tips in an FGM plate with a crack.

Functional gradation opens up new directions for optimizing both material and component structures to achieve high performance and material efficiency. At the same time, it posits many challenging mechanics problems, including the prediction and measurement of the effective properties, thermal stress distributions, and fracture of FGMs. The modeling and evaluation of the effective properties of FGMs has been considered in many works [11–13]. In [14], a comprehensive experimental and numerical study of the deformation and fracture of aluminum matrix–carbide particle composites was carried out. The applied numerical procedure could be useful for studying the fracture of ceramic/metal FGM structures. The evaluation of the fracture toughness of FGMs is also a very important problem for studying FGC fractures [15–18]. In [19], the analysis of the fracture parameters with respect to critical loads for a system of edge and internal cracks in FGCs showed the importance of taking into account the variation in fracture toughness through the thickness of the FGCs.

In our previous works [19–23], the theoretical study of the thermal and thermo-mechanical fracture of FGC/H structures was carried out under thermo-mechanical loading. These simulations were performed for different crack systems and geometries (edge crack systems [20], edge and internal cracks [21], edge and internal cracks imitating a curved interface [22]). Models for FGMs and some special models for cracks, such as partially thermally permeable cracks and cracks with contact, which could be used in the problem considered herein, were discussed in [23]. In [19–23], an exponential model of material properties was used. In the present work, the problem of the thermal fracture of FGM/H structures was investigated with the application of functions based on the rule of mixtures. To the best of the authors' knowledge, the problem of the interaction of arbitrarily located cracks in FGC/H structures with material properties described by functions based on the rule of mixtures has not been previously addressed.

Considering the possibility of optimizing an FGC in terms of improving its fracture toughness, material models based on the rule of mixtures are preferable. These models

contain a gradation parameter, which can be used to evaluate the profile of changes in the properties over the coating thickness. The rule of mixtures, originally applied to conventional composites, has been successfully used in FGMs [13,15]. The present work was devoted to the problem of the thermal fracture of FGC/H structures using functions based on the rule of mixtures. Emphasis was placed on the determination of critical stresses and the energy release rate near crack tips. One illustrative example is discussed for a system of interacting edge cracks in an FGC/H (PSZ/steel) structure.

2. Formulation of the Problem

In this theoretical work, the problem was considered for structures consisting of a functionally graded coating (FGC) of thickness h and an underlying homogeneous substrate (H), that is, for FGC/H structures, as shown in Figure 1. For thermal barrier coatings (TBCs), the top of the FG layer is made of a ceramic, a material with low thermal conductivity, and the homogeneous substrate is made of a metal. The FGC/H structure is cooled by ΔT , $\Delta T > 0$ (e.g., cooling from operating temperatures), and a tensile load p is applied parallel to the surface (see Figure 1).

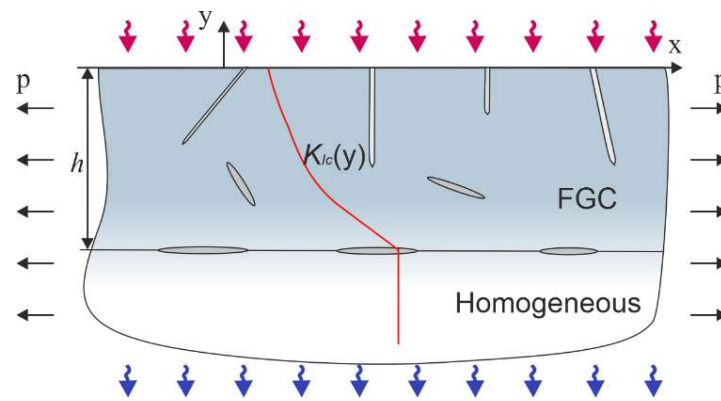


Figure 1. FGC/H structure with a system of cracks under the influence of thermal and mechanical loads. The fracture toughness $K_{Ic}(y)$ changes with the y -coordinate through the FGC thickness.

Pre-existing systems of cracks (length $2a_k$) in the FGCs were considered. A global coordinate system (x, y) with the x -axis lying on the FGC’s surface was introduced, and the local coordinates (x_k, y_k) refer to each crack, with the x_k -axis on the crack lines, as shown in Figure 2a. The position of cracks was determined explicitly by their midpoint coordinates (x_k^0, y_k^0) (or in the complex form $z_k^0 = x_k^0 + iy_k^0$, where i is the imaginary unit) and the inclination angles α_k to the x -axis, or β_k for edge cracks ($\beta_k = -\alpha_k$), see Figure 2a.

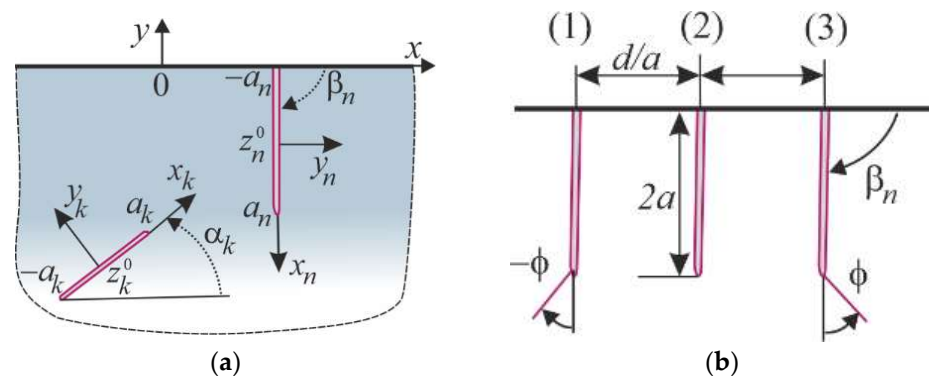


Figure 2. (a) Global (x, y) and local (x_k, y_k) coordinate systems; (b) three edge cracks.

The following assumptions were used for this problem. (1) The uncoupled, quasi-static thermo-elasticity theory was applied, i.e., that the temperature distribution is independent

of the mechanical field. (2) The thermal and mechanical properties of an FGC are continuous functions of the thickness coordinate y . (3) The non-homogeneity of the functionally graded material is revealed in the form of the corresponding inhomogeneous stress distributions on the surfaces of cracks [17,24,25]. These assumptions were also used in our previous works (e.g., see [19–23]).

3. Material Properties for FGCs and Residual Stresses

Due to the applications of TBCs and their requirements, in this study, only (ceramic/metal)/metal coatings were considered, that is, coatings in which the material composition varies with the y -coordinate from ceramic at the top of the FGC to metal in the substrate. Consequently, the thermal and mechanical properties of the FGC also vary continuously with the thickness coordinate y and can be mathematically described by a continuous function. It should be noted that this method is applicable to different material combinations.

In our previous works [19,21], an exponential form of Young's modulus and the thermal expansion coefficient was used, while in [23], a linear model was applied. The Poisson's ratio was assumed to be constant and equal to the value of the homogeneous substrate. Along with the change in these mechanical properties, the change in fracture toughness was also taken into account [19,21]. The importance of considering fracture toughness variation when determining critical stresses and assessing fractures was demonstrated in [19].

Another possibility for modeling FGC properties is the rule of mixtures, which with its various modifications has long been used for conventional composites. In contrast to conventional composites, in FGMs, the volume fraction of one material in relation to the other varies; thus, the effective properties for FGMs depend on the volume fraction of one material in relation to the other. In the present study, the thermal and mechanical properties as well as the fracture toughness (K_{Ic}) of the FGC were modeled by the rule of mixtures. The FGC consisted of two constituents, a ceramic on the top and a metal as a homogeneous substrate, with their volume fractions V_c and V_m , respectively, determined by a power law function:

$$V_m(y) = \left[\frac{y}{h} \right]^\lambda = \left[\frac{1}{h} \left(h + \text{Im} \left(z_n^0 \right) - x_n \sin(\beta_n) \right) \right]^\lambda, \quad (1)$$

$$V_c(y) = 1 - V_m(y) \quad (2)$$

with the power coefficient λ as the gradation parameter for the FGC. This parameter could be set to different values to realize different volume fractions as desired. The indices c and m refer to the volume of ceramic and metal, respectively. The case $\lambda = 0$ corresponds to a homogeneous material.

The material properties (the coefficient of thermal expansion and Young's modulus) of the functionally graded coating were assumed to take the following forms:

$$\alpha_t(y) = \frac{\alpha_{tm} V_m(y) E_m / (1 - \nu) + \alpha_{tc} V_c(y) E_c / (1 - \nu)}{V_m(y) E_m / (1 - \nu) + V_c(y) E_c / (1 - \nu)}, \quad (3)$$

$$E(y) = E_c \left[\frac{E_c + (E_m - E_c) V_m(y)^{(2/3)}}{E_c + (E_m - E_c) \left(V_m(y)^{(2/3)} - V_m(y) \right)} \right] \quad (4)$$

These expressions for the effective properties were used by Noda et al. [13]. In Equation (3), ν is Poisson's coefficient.

The fracture toughness (K_{Ic}) for FGCs also varies with the coordinate y and can be determined using one of the models described in [13,15]. This change in $K_{Ic}(y)$ is schematically shown in Figure 1. In [19,21,22], the fracture toughness for an FGM was determined theoretically and used for calculations. In the present work, to determine the fracture toughness, function (4) was used, where E should be replaced by K_{Ic} .

The method of superposition was used to solve this problem, so that loads at infinity are reduced to the corresponding loads on the crack faces. Thus, the tensile load is reduced to the load p_n on the crack surfaces (see, e.g., [26]):

$$p_n = \sigma_n - i\tau_n = p(1 - \exp(2i\beta_n))/2 = pf(\beta_n) \quad (n = 1, 2, \dots, N) \tag{5}$$

Here, N is the number of cracks. Additionally, as the temperature changes, e.g., when the structure is cooled by ΔT , residual stresses arise due to the mismatch in the thermal expansion coefficients (σ_n^T). Furthermore, the change in E leads to residual stresses σ_n^e . Thus, in standard FGCs, the full load on the n -th crack consists of p_n , σ_n^T , and σ_n^e , where the index “ n ” denotes that the functions are written in the local coordinate system (x_n, y_n) connected with the n -th crack (see, [24]):

$$p_n^* = p_n + \sigma_n^e + \sigma_n^T = pf(\beta_n) + pf(\beta_n)[E(y) - 1] + Q[\alpha_t(y) - 1]E(y), \quad (n = 1, 2, \dots, N). \tag{6}$$

$$Q = \alpha_{t1}\Delta TE_1 \tag{7}$$

It is assumed that $p = Q$; otherwise, the additional loading parameter p/Q should be considered. E_1 and α_{t1} are the material parameters of the substrate, and $\alpha_t(y)$ and $E(y)$ are obtained from Equations (3) and (4), respectively.

4. Solution and Determination of Fracture Characteristics

The method of singular integral equations was used. The integral equations were formulated using the method of complex potentials (see, [26]). On the right side of the equations were the known functions for the loads (see Equation (6)), and the unknowns were the derivative of the displacement jumps on the crack lines. The equations were solved numerically using the method of mechanical quadrature, based on the Chebyshev polynomials [26]. As a result of this method, the system of singular integral equations was reduced to a system of algebraic equations, from which the unknown derivatives of the displacements jumps on the crack lines were determined. Then, the stress intensity factors near the crack tips were calculated.

A complete description of the singular integral equations for this problem, as well as their numerical solutions, is provided in [21,22] and is not repeated here. The present equations differ from those previously described only in the right-hand sides containing the load functions. In the present problem, these load functions were defined by Equations (6) and (7).

In the considered problem, the cracks are mainly under mixed-mode loading conditions. The mixed-mode loading is due not only to the applied thermal and mechanical loads, but also to the interaction of cracks and the gradation of the material. That is, both stress intensity factors, Mode I and Mode II, are generally not equal to zero. In this case, the cracks will deviate from their initial paths. For predicting crack growth and determining its direction, the criterion of maximum circumferential stresses [27] was applied in this study. According to this criterion, the crack deviation angle ϕ (or the so-called fracture angle, see Figure 2b) and the critical stress intensity factors were calculated using the following relations:

$$\phi_n = 2\arctan \left[\left(K_{In} - \sqrt{K_{In}^2 + 8K_{II n}^2} \right) / 4K_{II n} \right], \tag{8}$$

$$K_n^{eq} \equiv \cos^3(\phi_n/2)(K_{In} - 3K_{II n} \tan(\phi_n/2)) = K_{Ic, tip} \text{ or } K_n^{eq} = K_{Ic, tip} \tag{9}$$

Equation (9) shows that crack growth occurs as soon as the equivalent stress intensity factor K_n^{eq} reaches the fracture toughness K_{Ic} . From Equation (9), the critical loads were obtained as follows:

$$\frac{P_{crn}}{p_0} = \frac{K_{Ic,n \text{ tip}}}{\cos^3(\phi_n/2)(k_{In} - 3k_{IIIn} \tan(\phi_n/2))} \frac{\sqrt{a}}{\sqrt{a_n}} \tag{10}$$

where $p_0 = K_{Ic1} / \sqrt{\pi a}$ is the critical load for a single reference crack subjected to a load p normal to the crack line with the stress intensity factor $K^0 = p\sqrt{\pi a}$ and $a = \max_{n=1, \dots, N} a_n$ ($n = 1, 2, \dots, N$, where N is the number of cracks). For an FGM, K_{Ic} is defined by an expression similar to Equation (4).

In Equations (8)–(10), the dimensional and non-dimensional stress intensity factors (SIFs) are related as follows:

$$K_{In} - iK_{IIIn} = p\sqrt{\pi a_n}(k_{In} - ik_{IIIn}) \tag{11}$$

The fracture angle ϕ_n is shown in Figure 2b. First, the angle of the crack propagation (fracture angle, Equation (8)) was obtained. Then, the critical loads were calculated near the crack tips (Equation (10)). Finally, the weakest crack was defined by the following conditions:

$$P_{cr} = \min_n P_{crn} / p_0 \quad (n = 1, 2, \dots, N).$$

In the present work, attention was mainly paid to the determination of critical loads for systems of interacting cracks in an FGC. Crack path predictions (based on fracture angles) for other material models were investigated, e.g., in [22].

Another fracture characteristic that is particularly useful for studying fracture in FGCs is the energy release rate:

$$\frac{G_n}{G_0} = \left[k_{In}^2 + k_{IIIn}^2 \right] \frac{a_n}{a} \cdot \frac{E'_1}{E'(y)} \tag{12}$$

where E' represents E for the plane stress and $E/(1-\nu^2)$ for the plane strain state; E_1 is the Young's modulus of the substrate; $E(y)$ is given in Equation (4); the energy release rate G_0 refers to a single reference crack; and the non-dimensional stress intensity factors k_I and k_{II} are defined in Equation (11).

5. Results

As an illustrative numerical example, consider three edge cracks as shown in Figure 2b. The results were obtained for the following parameters: $d/a = 4.0$, $h/a = 4.0$, $2a$ —crack size; $\Delta T = 300^\circ\text{C}$. The thermal load Q is defined by Equation (7). The material parameters are listed in Table 1 and were taken from [28], where further useful references can be found.

Table 1. Material parameters.

Material Property	Top Coat (Ceramic)—PSZ	Bottom Coat (Metal)—Steel
Young's modulus (GPa)	48.0	207.0
Fracture toughness (MPa m ^{1/2})	7.0	50.0
Thermal exp. coeff. (10 ⁻⁶ K ⁻¹)	9.0	15.0

The normalized critical loads p_{cr}/p_0 as functions of the inclination angle β ($\beta_n = \beta$, $n = 1, 2, 3$) are shown in Figure 3. Figure 3a,b present the results for three FGM models: exponential, linear, and the rule of mixtures. Figure 3c,d present the results for the rule of mixtures for different λ values (0.1, 0.9, 1.9, and 2.9). Figure 3a,c refer to crack 1, and Figure 3b,d refer to the middle crack 2 (see geometry in Figure 2b). The fracture characteristics for crack 3 were similar to those of crack 1 and are not shown in the figures. The largest value for p_{cr}/p_0 was for crack 2, and the smallest was for crack 1; thus, a

shielding effect was observed for crack 2. The lowest p_{cr}/p_0 value was for the rule of mixtures model (for $\lambda = 1$), as seen in Figure 3a,b. The p_{cr}/p_0 increased with increasing λ , and for $\lambda = 2.9$, the values were close to p_{cr}/p_0 for the exponential model (compare Figure 3a,c for crack 1, and Figure 3b,d for crack 2).

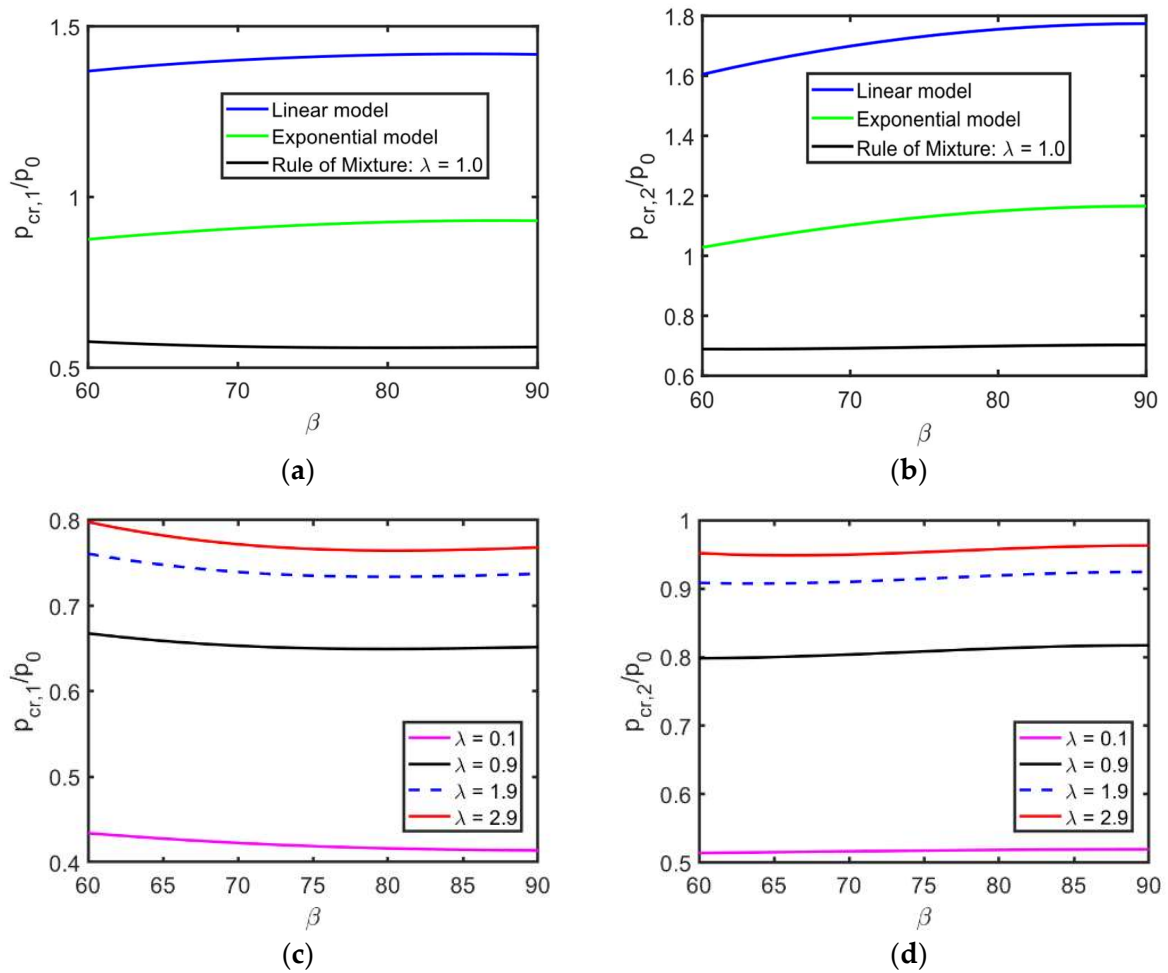


Figure 3. Critical loads as a function of β : (a,b) for three FG models; (c,d) for the rule of mixtures for different values of λ (0.1, 0.9, 1.9, and 2.9); (a,c) for crack 1 and (b,d) for middle crack 2.

Different values of the critical load for different material models (as seen in Figure 3) but the same crack showed a difference in the fracture toughness values determined by these models, which in turn showed different concentrations of ceramic (metal) near the crack tip. Different models (or different values of the gradation parameter λ in the rule of mixtures model) provided different profiles of material change, which meant different K_{Ic} values near the crack tip. As can be seen from Equation (10), p_{cr}/p_0 depended on K_{Ic} .

Ceramics in coatings create a thermal barrier and protect metal parts from overheating. The metal content in an FGC increases the strength of the FGC but reduces the thermal insulation. Thus, it is necessary to balance the content of ceramic and metal in coatings to improve the thermal insulation properties of FGCs.

Figure 4 depicts the effect of the thermal load Q on the energy release rate (ERR) (Figure 4a,b) and critical loads p_{cr}/p_0 (Figure 4c,d) for a wide range of grading parameter λ values (from 0.1 to 3.0) in the rule of mixtures model. The results are presented for crack 1 (Figure 4a,c) and middle crack 2 (Figure 4a,c); the cracks were inclined on 90° to the surface. The parameter ranges of thermal loading Q corresponded to a temperature change ΔT ($^\circ\text{C}$) from 300° to 400° .

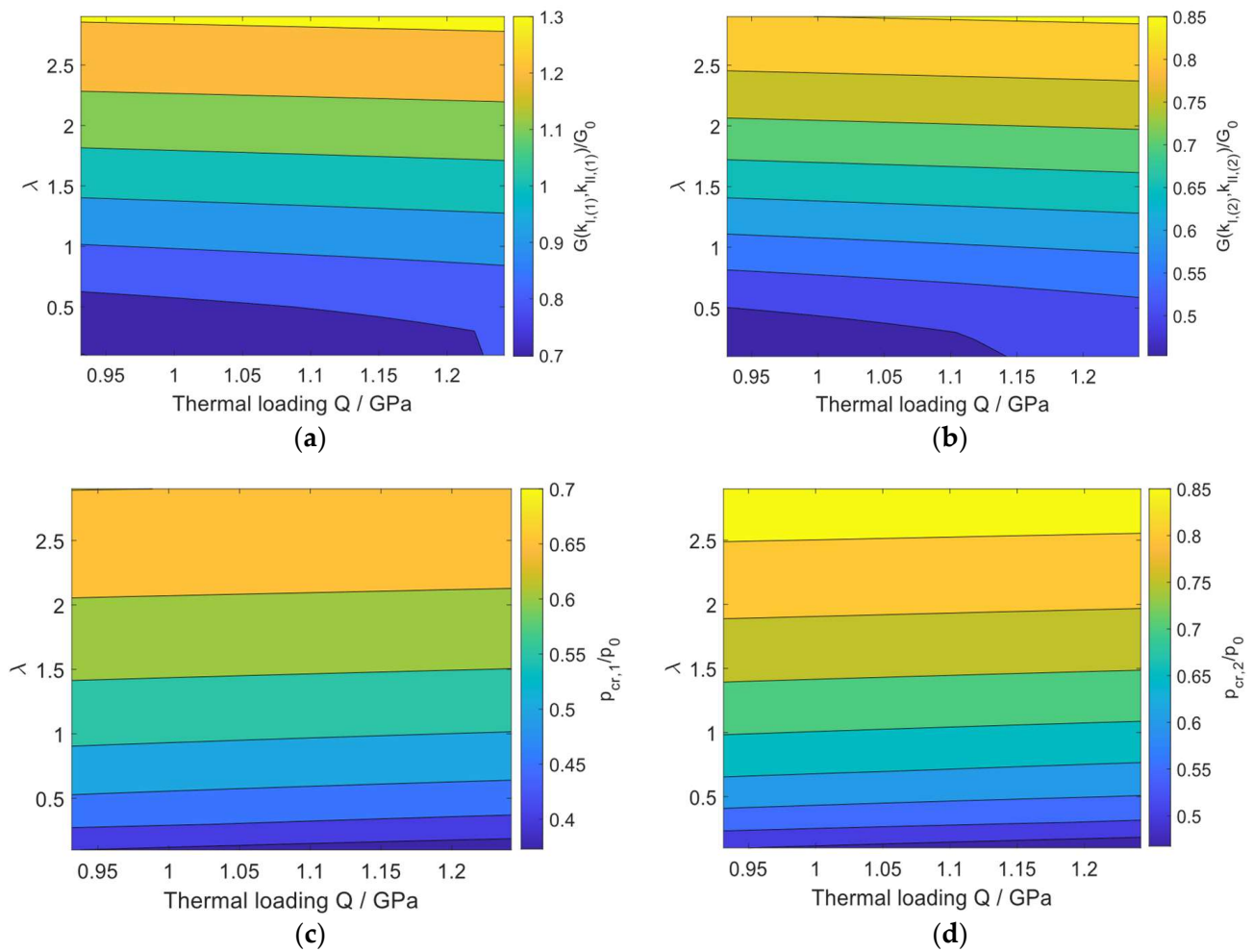


Figure 4. Influence of thermal loading Q and gradation parameter λ on ERR (a,b) and critical load (c,d); (a,c) for crack 1 and (b,d) for middle crack 2.

An increase in the thermal loading Q caused an increase in the energy release rate but decreased the critical load; that is, a reduction in the resistance to crack propagation was observed. This was due to the higher loading (additional residual stress) acting on the cracks.

The dependence of the fracture characteristics on λ was as follows: with an increase in the gradation parameter λ , both ERR and p_{cr}/p_0 increased. A higher gradation parameter corresponded to a higher metal content and a lower ceramic content in the FGC.

6. Conclusions

A theoretical study based on the method of singular integral equations was performed for FGC/H structures under thermo-mechanical loads. For the modeling of the material gradation of FGCs, functions based on the rule of mixtures were used. The structural variation of fracture toughness in FGCs was also taken into account and was shown to play an important role in evaluating fracture characteristics, especially critical loads. An illustrative example of three edge cracks in an FGC was studied in detail to investigate the influence of the material and geometrical parameters of the problem on the fracture characteristics of interacting cracks. The weakest cracks in the considered system of three edge cracks were the outer edge cracks in the FGC/H (ceramic/metal)/metal structure. A shielding effect was observed for the middle crack. For the rule of mixture model, it was observed that the variation in gradation parameter λ led to a significant change in the fracture parameters, in particular, the critical loads and energy release rates.

The above results for critical loads and energy release rates demonstrate their strong dependence on the gradation parameter λ for different combinations of materials in coatings. Thus, this model is a good candidate for a theoretical evaluation of the desired material properties of FGCs for their further development in order to improve the thermal fracture resistance of coatings.

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