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A generalized *J*-integral for thermal shock analyses of 3D surface cracks in spatially and temperature dependent materials

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ABSTRACT

Thanks to their favorable mechanical properties and modern manufacturing technologies, functionally graded materials (FGM) and structures have gained increasing utilization in engineering. One major applications of functionally graded ceramics, refractories or heat protecting layers is to improve the resistance against thermal shock impact. Here, fracture mechanical methods are needed to evaluate the strength and durability of such structures exposed to transient thermomechanical loading. Despite a lot of theoretical work has been done for two-dimensional crack configurations in thermoelastic FGM, real defects and structural components are of three-dimensional (3D) nature. In most cases the real gradation of the thermoelastic material properties does not obey simple mathematical functions, but shows a complex physical dependency on location due to manufacturing. Moreover, the elastic and thermodynamic properties depend on temperature itself.

In this paper, we present the derivation of the 3D *J*-integral for arbitrary location and temperature dependent anisotropic material behavior. The functionally varying material properties are implemented in the finite element method (FEM) by means of »graded elements«. The *J*-integral is calculated in post-processing using the equivalent domain integral technique. The method is applied to surface cracks in a functionally graded plate under mechanical and thermal shock loading. Hereby, the real measured variation of all thermal and mechanical properties with porosity and temperature is exploited for a CaAl ceramic. The influence of the material gradation on the fracture parameters J and K_I is investigated in various examples in order to find optimal gradation functions. It could be shown that the temperature dependency of thermoelastic material properties has an important effect on the results and must not be neglected.

1. Introduction

Due to their favorable mechanical properties, functionally graded materials (FGM) and structures have gained increasing engineering applications, e.g. in thermal barrier coatings, refractory materials or transition layers between dissimilar materials. Meanwhile, there exist several technologies to manufacture graded structures like additive printing, laser sintering, co-firing, tape casting, and spraying of coatings. The motivation for the present study was the development of new refractory ceramics made by graded or layered materials to get improved thermal shock resistance for metallurgical applications, see the special issue [1]. Under service conditions, FGMs are often exposed to transient temperature fields by thermal shock loading. One problem, especially with ceramic FGM, is their inherent brittleness, which requires fracture mechanical concepts to ensure safety and residual strength under thermomechanical loading. In order to evaluate the stress state at cracks in FGM, several analytical and finite element techniques (FEM) have been developed. The solution requires a staggered thermomechanical analysis, whereby the transient temperature field is firstly obtained from a thermal analysis. Afterwards the temperature fields are employed as loading condition in a subsequent thermoelastic stress analysis step. In both simulations the spatial gradation and the temperature dependence of material properties have to be taken into account.

In the literature, at first thermal shock loading of cracks in two-dimensional (2D) FGM has been analyzed, see for example [2–6]. There exists a plenty of articles dealing with methods to compute fracture mechanical loading parameters as stress intensity factors, energy release rates, variants of *J*-integrals, etc. An overview can be found in [7,8]. Most of them consider two-dimensional (2D) crack problems.

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Nomenclature

$\alpha_{ij}^{\mathrm{th}}$	tensor of thermal expansion coefficients
δ_{ij}	Kronecker symbol
ε_{ij}	strain tensor consisting of mechanical $\varepsilon_{ij}^{\mathrm{m}}$ and thermal strain tensor $\varepsilon_{ij}^{\mathrm{th}}$
λ	heat conduction coefficient
λ_L, μ_L	Lame's elastic constants
ϱ	density
Φ	synonym for a material property
σ_{ij}	stress tensor
ΔA	virtually extended crack area along a crack segment Δs
Δl_m	virtual crack propagation vector
a	crack length
C_{ijkl}	elasticity tensor
c	half crack width
c_{m}	mass specific heat capacity
E	Young's modulus
f_{P}	amount of pore forming agents in the ceramic
G	energy release rate
J_m	J-integral vector
$\bar{J}$	released energy (related to virtually extended crack area ΔA)
n_i	unit normal vector on integration contour
q, q_{m}	smoothly varying weighting function
$\bar{q}_s$	external heat flux on surface
s	crack front position
T_0, T	(initial) temperature field
t_i	traction vector $t_i = \sigma_{ij} n_j$
U	strain energy density
u_i	displacement vector
v_i	direction vector of crack propagation
x_i	coordinate vector
EDI	equivalent domain integral
FEM	finite element method
FGM	functionally graded material

Without any claim to completeness, the following short literature review is restricted to thermomechanical crack analyses in FGM and the development of enhanced formulations of the J-integral concept. Eischen [9] seems to be the first who developed a domain independent J_k-integral vector to compute mixed-mode stress intensity factors for nonhomogeneous cracked bodies. In their pioneering work, Kim and Paulino [10,11] presented basic concepts for applying FEM to 2D crack analysis in isotropic and orthotropic FGMs under mechanical loads. They have calculated 2D mixed-mode SIFs in FGMs by means of the path-independent J_k-integral using the equivalent domain integral (EDI). Dag [12] formulated a 2D version of J_k-integral to compute mixed-mode fracture parameters for cracks that are inclined to the direction of material property gradation in FGMs under action of thermal stresses.

For 3D crack problems, Walters et al. [13] provided the basic formulations of the equivalent domain form of the J-integral under stationary thermomechanical mode I loading. Yildirim et al. [14] employed a displacement interpretation technique when studying semi-elliptical surface cracks in a coating subjected to transient thermal loading. Ayhan [15,16] and Dag et al. [17] used enriched element functions, which allow to compute the stress intensity factors directly from the FE solution along the crack front under mixed-mode-loading. This way, post-processing techniques like displacement interpretation, virtual crack closure integrals (VCCI), J-integrals or interaction-integral become no longer necessary. To investigate non-planar crack shapes subjected to steady state temperature gradients, Moghaddam and Alfano [18] employed the interaction integral method to differentiate between mode I and mode II K-factors. Nami and Eskandari [19] used the simple displacement interpretation method to calculate the stress intensity factors for a semi-elliptical surface crack in a FGM cylinder under pressure and steady state thermal fields.

Regarding the numerical requirements to solve the heat conduction and thermoelastic problem for FGM with the FEM, often an approximation by means of many thin layers is applied in the literature, see e.g. [4,5]. Usually, in commercial FEM-codes only homogeneous material properties are assigned to every finite element. In order to avoid numerical errors in the solution at the element boundaries, a fine mesh is inevitably required. Another approach has been pursued by Kim and Paulino [20,21], Yildirim and Erdogan [22] as well as KC and Kim [23] for 2D problems and by Walters et al. [13] for 3D thermoelastic problems. These authors developed special »graded« finite elements with shape functions that take an inhomogeneous material distribution into account. This technique is adopted by the present authors, see details in Section 2.4.

In most of the fracture analyses presented in the literature for FGMs, simple mathematical (exponential, polynomial, etc.) functions were arbitrarily chosen for the spatial gradation. This is regarded as a severe simplification, since the real physical causes and interdependencies for gradation of the different properties are not elucidated. Therefore, here true measured relationships are used for porous ceramics, reflecting the effect of pore forming agents on all relevant mechanical and thermal material properties. As another novelty, the strong dependence of thermomechanical material properties of FGM on temperature is taken into account, which is regarded as necessary for thermal shock scenarios.

The mathematical writing in this paper uses the tensor index notation with summation convention. A comma after an item $(\cdot)_{,i} = \partial(\cdot)/\partial x_i$ denotes partial differentiation with respect to coordinate x_i. δ_{mj} means Kronecker's unity tensor.

2. *J*-integral for location and temperature dependent materials

2.1. Basic formulation of J-integral vector

We start the derivation from the classical J-integral as developed by Rice and Cherepanov for two-dimensional (2D) elastic problems. The J-integral is defined as a line integral along a contour C_{C} around the crack tip, see Fig. 1.

$$J = J_1 = \lim_{r \to 0} \int_{C_{\mathrm{C}}} \left(U(x_i, \varepsilon_{ij}^{\mathrm{m}}, T) n_1 - t_i u_{i,1} \right) \mathrm{d}s \tag{1}$$

Hereby, $U(x_i, \varepsilon_{ij}^{\mathrm{m}}, T)$ is the elastic strain energy density as function of the elastic strain $\varepsilon_{ij}^{\mathrm{m}}$, the temperature T and in case of materials gradation of coordinate x_i as well. $t_i = \sigma_{ij} n_j$ denotes the traction vector on the contour derived from the stress tensor σ_{ij} and the outward normal vector n_j. The total strains are composed from elastic and thermal parts $\varepsilon_{ij} = \varepsilon_{ij}^{\mathrm{m}} + \varepsilon_{ij}^{\mathrm{th}}$.

The physical meaning of J is the energy release rate in case of a crack propagation in x_1-direction: $G = J = J_1$. In its strong sense this relation is only valid for an infinitesimal small contour C_{C} around the crack tip $\lim_{r \to 0}$. For location and temperature dependent

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