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Multiple Surface Cracking and Debonding Failure for Thin Thermal Coatings

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Abstract

A mechanical analysis of thin films of quasi-brittle materials used as thermal coatings for superalloy substrate is proposed. The study considers a bi-material element subjected to uniform tension formed by a thin layer of quasi-brittle material (typically a ceramic) bonded on an elastic substrate. The bounding between the coating film and the substrate is realized by a very thin primer which mechanically modeled as a zero thickness cohesive frictional interface. The analysis is developed by a non-linear finite element simulation in which, in order to consider damage size effects, a non-local isotropic damage model is adopted for the quasi-brittle coating. The results of the analysis shows the formation of multiple cracks on the coating surface which propagate up to the interface. At the same time, due to the mismatch between the elastic moduli between the coating and the substrate and the development of the transverse cracks, a competing debonding mechanism along the interface develops. The numerical results show also, for thick coating layers, the development of skew crack bands, which forecast coating spalling.

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Keywords: Multiple cracks; damage localization; cohesive interface.

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1. Introduction

Superalloy mechanical components working under high temperature cycles, such as blades of gas turbines of aircraft engines, or high performance electricity generators, are usually thermally shielded by thin coating layers of ceramic-type materials. Mechanical tests for small scale superalloy beams with a thin thermal coating, have shown complex failure mechanisms (McGuigan et Al. (2003); Chen et Al. (2011); Peng et Al. (2018)).

The failure are mainly characterized by the combination of surface tensile cracks, which forms on the external coating surface and then propagates in the interior up to the interface with the superalloy, and a shear debonding mechanism developing along the interface between the superalloy and the coating. The ultimate failure is characterized by the mechanical expulsion of pieces of coating which leaves the superalloy unprotected and then prone to very high thermal strains and therefore severe damage and possibly overall failure.

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Few analytical results, under simplified hypothesis, are available for this type of problem. For instance, if it is assumed a uniaxial state and full adhesion between the two elements, it is possible to evaluate the distance between longitudinal cracks (McGuigan et Al. (2003)). Alternatively the debonding can be analyzed following a strategy similar to the one proposed in Alessi et Al. (2017).

The present contribution investigates the above problem by a nonlinear computational approach based on incremental finite elements simulations. The substrate is modelled as a elastic material with an high stiffness, typical for superalloys, which however need to operate inside a certain temperature range for not suffer of changes in the solid state, which may produce in turn lower mechanical performance. The thin film of ceramic material, which play the role of thermal coating, is modeled as a quasibrittle material with elastic-damage constitutive relations. Elastic damage constitutive relations need to be regularized in order to maintain the well posed features essential for meaningful numerical analyses. In the present contribution the thin layer is modeled by a nonlocal damage model, similar to the one proposed by the authors in Borino et Al. (2009). In this way the formation and propagation of cracks is naturally reproduced by the localization of damage in narrow bands which, however maintain a finite width and then keep the overall finite element problem well posed and mesh objective. The last nonlinear mechanism describes the decohesion between the thin coating and the substrate and it is modeled by a zero-thickness cohesive-frictional mechanical interface (Parrinello et Al. (2015, 2016)).

A coupling between nonlocal damage and interface has been previously proposed by Marfia et Al. (2011) for the analysis of FRP bounded on damageable substrate. Alternatively a coupling between phase field model and mechanical interface has been also propose by Paggi and Reinoso (2017)

In this contribution a few 2D nonlinear finite elements simulation are proposed showing the multiple damage localization patterns on the coating surface. A discussion on the amplitude and distance between these surface cracks is presented. The formation and propagation of the decohesion at the interface is also analyzed. Finally some design consideration on the optimal thickness of the coating and the most efficient thermal barrier from a mechanical point of view is discussed.

2. The bi-material element in tension

The structural element considered for the analysis is a bi-material element of length L in plane strain condition, subjected to a uniform tensile load to one end and fixed to the other end (see Fig. 1).

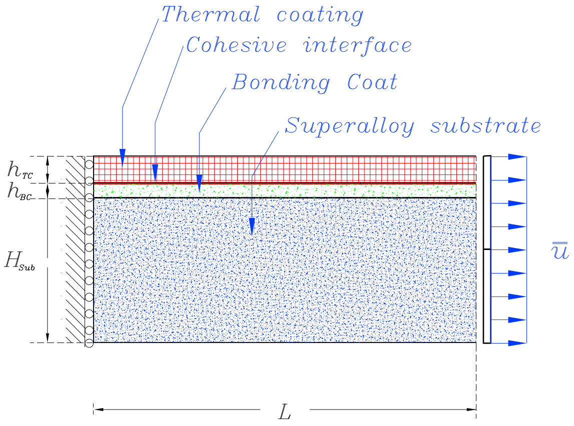

Fig. 1. Sketch of the bi-material structural element composed by an elastic superalloy substrate and a quasi-brittle thermal coating. The two layers are connected by a mechanical cohesive-frictional interface.

The element is composed by a substrate of thickness h_s, which is a superalloy assumed to remain in a pure elastic regime during the loading.

The coating layer, of thickness h_c is typically composed by a ceramic material which is assumed to behave constitutively as a quasi-brittle material.

Continuum damage models can effectively be adopted for modeling the constitutive response of the coating layer. Damage models typically produce, at same loading stage, strain localization, which are the source of formation and propagation of cracks. In order to mantain mesh objective results regularization techniques are required such as: nonlocal damage models Bažant and Jirásek (2002); Borino et Al. (2009), gradient damage models Vandoren and Simone (2017), or following more recent trends phase field approach Giambanco and La Malfa Ribolla (2019).

Between the substrate and the coating a bond coating very thin layer is inserted which could be a Ni foil, which plays the role of primer for the adhesion an it also works as a corrosion barrier for the superalloy (Zhu et Al. (2015)). Because of the very small thickness of the bonding layer and since it is the locus of the final failure for delamination this element is modeled as a zero thikness cohesive frictional mechanical interface. Mechanical interface models are largely employed for modeling cohesive fracture problem, especially when the spatial locus where formation and possible propagation of fractures is known a-priori. The literature concerning interface mechanical models is rather rich (Parrinello et Al. (2009); Giambanco et al. (2012); Parrinello et Al. (2015); Scimemi et Al. (2014); Serperi et Al. (2015))

2.1. *The nonlocal damage model for the coating*

The constitutive model adopted to reproduce the mechanical response of the thermal coating is a nonlocal damage model based on the formulation proposed in Borino et Al. (2009). The model adopted is a symmetric formulation thermodynamically consistent and allow to introduce in the constitutive formulation an internal length parameter ℓ which takes into account the effect of the microstructure dimension into the spatial spread of the damage band. The nonlocal damage is then able to predict a strain localization of a finite thickness related to the material microstructure and therefore the relevant size effect.

The elastic damage stress-strain relation reads

$$\boldsymbol{\sigma}(\boldsymbol{x}) = (1 - \bar{\omega}(\boldsymbol{x}))\,\boldsymbol{E}\,\boldsymbol{\varepsilon}(\boldsymbol{x}) \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{E}$ is the material elastic moduli tensor, $\boldsymbol{\varepsilon}$ is the infinitesimal strain tensor and $\bar{\omega}$ is a nonlocal measure of the isotropic scalar damage space distribution ω. Namely, $\bar{\omega}$ is a space weight average of the local damage ω obtained as

$$\bar{\omega}(\boldsymbol{x}) \int_V W(\boldsymbol{x},\boldsymbol{y})\,\omega(\boldsymbol{y})\,dV(\boldsymbol{y}) \tag{2}$$

The spatial weight function $W(\boldsymbol{x},\boldsymbol{y})$ is given as

$$W(\boldsymbol{x},\boldsymbol{x}) = \left(1 - \frac{\Omega_r(\boldsymbol{x})}{\Omega_\infty}\right)\delta(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{\Omega_\infty}\,\exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|^2}{2\ell^2}\right) \tag{3}$$

The function W is a sum of two contribution. Since $\delta(\boldsymbol{x})$ is the Dirac delta function, the first is a strictly local part which gives a contribution at point close (with respect to the internal lengnt ℓ) to the boundary of the body V and tend to vanish for points far from the boundary. The second part is characterized by an exponential function which depends on the relative distance $r = \|\boldsymbol{x}-\boldsymbol{y}\|$ ad becomes dominant for points of the body far from the boundary of V. The function Ω_r id defined as

$$\Omega_r(\boldsymbol{x}) = \int_V \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|^2}{2\ell^2}\right) dV(\boldsymbol{y}) \tag{4}$$

and constant Ω_∞ is the value of the integral given in eq.(4) when the integration is performed on the unbounded 2D domain. The weighting function W, defined in eq.(3), is symmetric with respect to $\boldsymbol{x}, \boldsymbol{y}$ at any point in V and satisfy the following normality condition:

$$\int_V W(\boldsymbol{x}, \boldsymbol{y})\, dV(\boldsymbol{y}) = 1. \tag{5}$$

Beside the constitutive relation (1) a nonlocal damage activation function is defined as

$$\phi_d(\bar{Y}, \chi) = \bar{Y} - \chi - Y_0 \leq 0 \tag{6}$$

where

$$\bar{Y}(\boldsymbol{x}) \int_V W(\boldsymbol{x}, \boldsymbol{y})\, Y(\boldsymbol{y})\, dV(\boldsymbol{y}) \tag{7}$$

where Y is the energy release rate, χ is an internal variable able to characterize the post peak stress-strain softening material response and Y_0 is the initial damage activation threshold.

$$Y = \frac{1}{2} \boldsymbol{\varepsilon}^T \boldsymbol{E}\, \boldsymbol{\varepsilon} \tag{8}$$

Following a damage softening law proposed by Comi and Perego (2004), the internal variable χ is related to the damage ω by the following state law

$$\chi = \kappa \ln^n \left(\frac{c}{1 - \omega} \right) - \kappa \ln^n c \tag{9}$$

where κ, n, c are parameters that describes the post elastic stress-strain response. With reference to the uni-axial response it is possible to identify the constant by the following relations (Comi and Perego (2004))

- Damage threshold: $Y_0 \equiv 1/2E\varepsilon_e^2 = \kappa \ln^n c$
- Fracture Energy $G_f = Y_0 + cn\kappa \exp[-(Y_0/\kappa)^{1/n}](n-1)! \sum (1/i!)(Y_0/\kappa)^{i/n}$

The constant $c \geq 1$ is related to the stress-strain slope at the final elastic strain ε_e, and for $c = e^{n/2}$ an initial horizontal slope is achieved followed by negative slope, i.e. softening.

The damage flow rules and the loading/unloading conditions complete the nonlocal damage constitutive framework:

$$\dot{\omega} = \frac{\partial \phi_d}{\partial \bar{Y}} \dot{\lambda} = -\frac{\partial \phi_d}{\partial \chi} \dot{\lambda} \tag{10}$$

$$\dot{\lambda} \geq 0, \qquad \phi_d \leq 0, \qquad \dot{\lambda} \phi_d = 0. \tag{11}$$

2.2. *The interface model*

In order to describe the development of discontinuities in the displacement at the bounding region between the substrate and the thermal coating layer (debonding) a mechanical interface is introduced. The interface model adopted for the analysis is a recent evolution of a thermodynamically consistent mixed-mode cohesive-frictional interface model developed by the authors (Parrinello et Al. (2015, 2016); Parrinello and Borino (2018, 2019)).

The interface model is based on the assumption that the dechoesion surface can be decomposed in two fractions related to the value of a surface damage variable ω_s. Namely, a creaked fraction $\omega_s\, dS$ and a sound fraction $(1-\omega_s)\, dS$. The traction vector across the interface $\boldsymbol{t}$ is therefore given as a sum of the two contributions $\boldsymbol{t} = \boldsymbol{t}_s + \boldsymbol{t}_c$ with

$$\boldsymbol{t}_s = (1-\omega_s)\boldsymbol{K}_s\boldsymbol{\delta}_s^e; \qquad \boldsymbol{t}_c = \omega_s\boldsymbol{K}_c\boldsymbol{\delta}_c^e \tag{12}$$

where $\boldsymbol{K}_s$ and $\boldsymbol{K}_c$ are the diagonal stiffness matrices of the two interface fraction and $\boldsymbol{\delta}_s^e$ and $\boldsymbol{\delta}_c^e$; are respectively the interface displacement discontinuity vectors for the two fractions. Two activation functions are introduced for the description of both mode I (opening), mode II (sliding) and any mixed mode. The first is a damage activation function:

$$\phi_d^s = Y_s - \chi_s - \tilde{Y}_{s0}(\boldsymbol{u}) - Y_{s0} \leq 0 \tag{13}$$

where Y_s is the surface energy release rtate given as

$$Y_s = \frac{1}{2}\boldsymbol{\delta}_s^{eT}\boldsymbol{K}_s\boldsymbol{\delta}_s^e - \frac{1}{2}\boldsymbol{\delta}_c^{eT}\boldsymbol{K}_c\boldsymbol{\delta}_c^e \tag{14}$$

In eq.(13) Y_{s0} is the initial threshold for the surface damage activation, χ_s is the internal variable that drive the interface softening state and finally $\tilde{Y}_{s0}(\boldsymbol{u})$ is a positive term which allows to drive fracture mixity.

A second activation function is introduced, which takes into account the frictional behavior in the form of a Mohr-Coulomb yield function

$$\phi_p^s(\boldsymbol{t}_c) = |t_{ct}| + \alpha t_{cn} \leq 0 \tag{15}$$

where α is the frictional coefficient and t_{ct} and t_{cn} are the tangential and normal components of the traction vector $\boldsymbol{t}_c$ which acts on the damaged fraction and can generate frictional effects even before that the interface is fully damaged. The interface damage flow rule reads

$$\dot{\omega}_s = \frac{\partial\phi_d^s}{\partial\bar{Y}_s}\dot{\lambda}_s = -\frac{\partial\phi_d^s}{\partial\chi_s}\dot{\lambda}_s \tag{16}$$

and regarding the frictional displacements

$$\dot{\delta}_n^p = \frac{\partial\psi_p}{\partial t_{cn}}\dot{\lambda}_p = sgn(t_{ct})\dot{\lambda}_p \qquad \dot{\delta}_t^p = \frac{\partial\psi_p}{\partial t_{ct}}\dot{\lambda}_p = \beta\dot{\lambda}_p \tag{17}$$

where ψ_p is the interface frictional potential given as

$$\psi_p(\boldsymbol{t}_c) = |t_{ct}| + \beta t_{cn} \tag{18}$$

in which $\beta \leq \alpha$ is the dilatancy coefficient.

The damage interface constitutive formulation is completed by the loading unloading conditions

$$\dot{\lambda}_s \geq 0, \quad \phi_d^s \leq 0, \quad \dot{\lambda}_s \phi_d^s = 0; \qquad \dot{\lambda}_p \geq 0, \quad \phi_p^s \leq 0, \quad \dot{\lambda}_p \phi_p^s = 0; \tag{19}$$

3. Numerical Analysis

The formulation presented in the previous Sections has been implemented in the open source finite element code FEAP. The structural element of Fig. 1 has been discretized by 9-node plane strain . The length of the specimen is L = 10 mm. The thickness of the substrate is $h_s = 1.5$ mm. Two different thickness for the thermal coating layer has been considered. The first is a thin coating $h_c^{(1)} = 0.2$ mm, whereas the second is a thick coating of $h_c^{(2)} = 0.6$ mm.

The substrate is considered as an isotropic linear elastic material with elastic modulus $E_s = 200$ GPa and Poisson ration $\nu_s = 0.3$

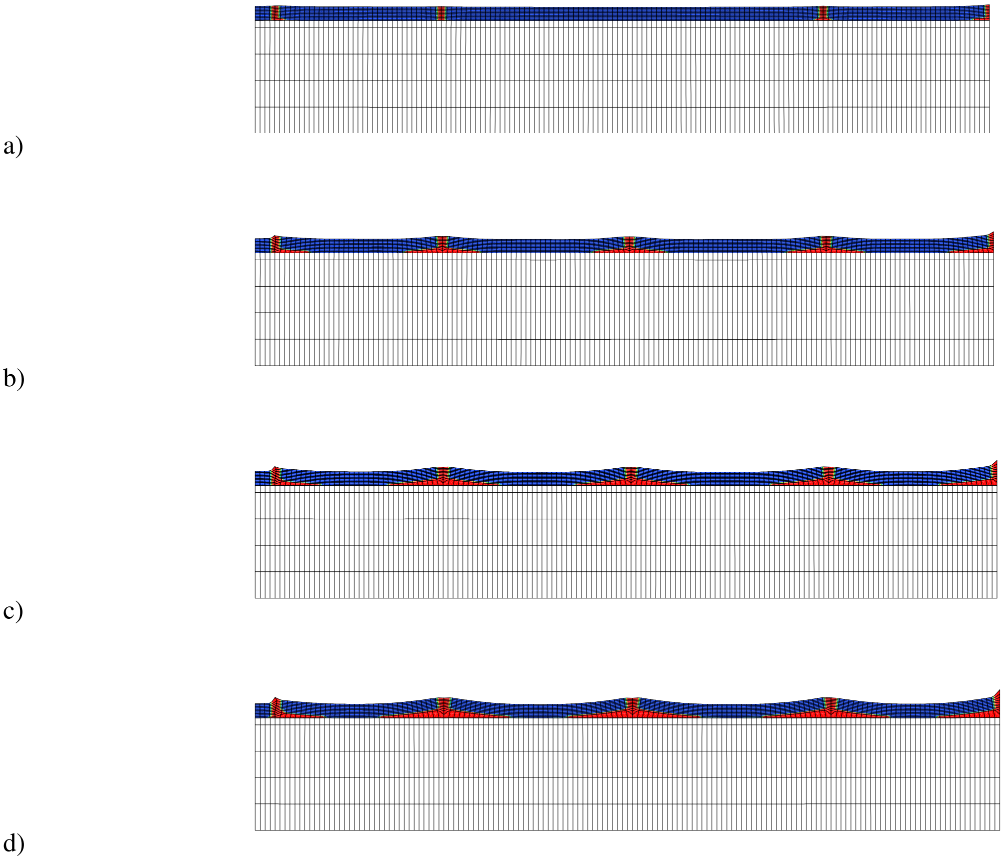

Fig. 2. Damage distribution at the thin thermal coating for increasing loading stages from a) to d).

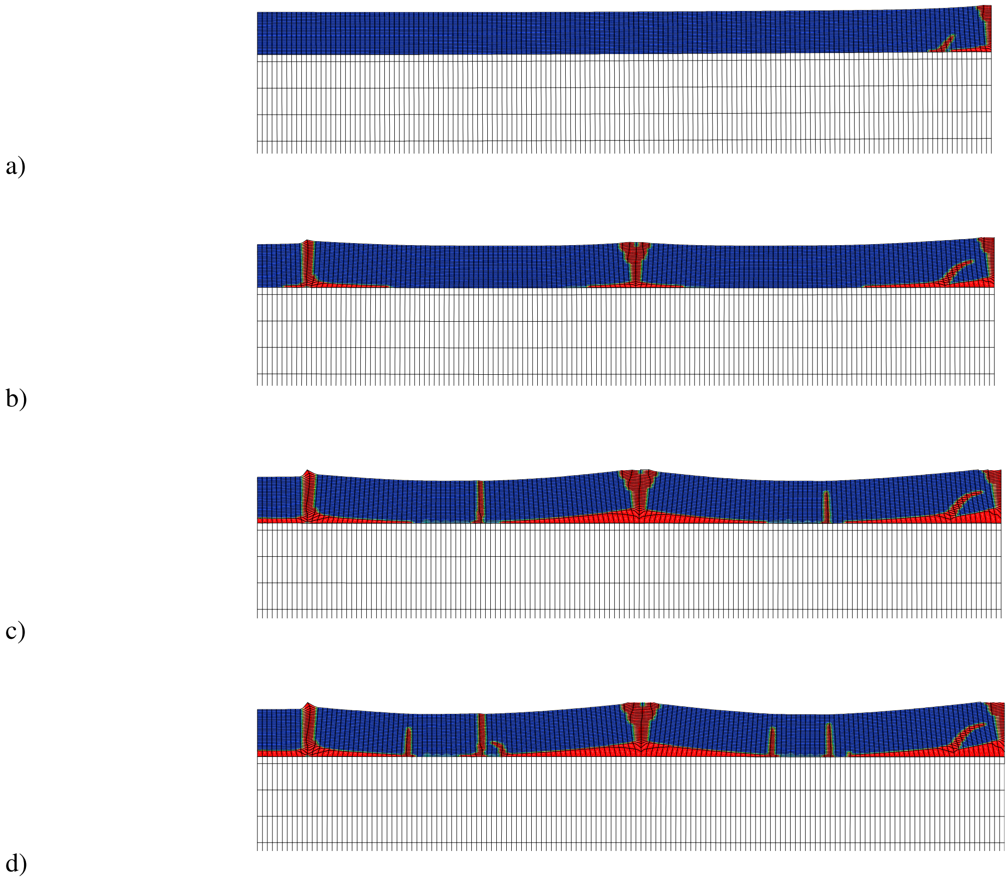

Fig. 3. Damage distribution at the thin thermal coating for increasing loading stages from a) to d).

The thermal coating has been considered as a nonlocal elastic damage material following the model of Sec. 2.1. The material data adopted are:

- Elastic modulus $E_c = 25$ GPa
- Poisson ratio $\nu_c = 0.3$
- Damage parameters $c = 2.7182$; $\kappa = 0.018$; $n = 2$.
- damage internal length $\ell = 0.02$ mm

In order to allow dechoesion mechanisms between the substrate and the thermal coating, a zero-thickness cohesive-frictional 6-node interface elements have been inserted. The model adopted is the one described in Sec. 2.2. with the following constitutive parameters:

- Normal and tangential interface stiffness $K_n = K_t$ 50 kN/mm
- Fracture Energies $G_I = G_{II} = 0.3$ N/mm
- Elastic normal traction limit $t_{0n} = 20$ N.
- Friction coefficient and dilatancy coefficient $\alpha = \beta = 30^0$

The incremental nonlinear finite element responses are discussed in next Subsections.

3.1. Thin coating results

For the structural element with the coating of thickness $h_c^{(1)} = 0.2$ mm, the results in terms of damage distribution at different loading levels are reported in Fig. 2. It emerges that after the formation of the first vertical crack in the coating, a second crack is formed at a distance $L_{c)}$. Increasing the impressed displacement a further vertical crack is formed at mid distance $L_{(c)}/2$ between the previous two cracks. The development of further cracks at the mid distance $L_{(c)}/4$ is then observed. This development of vertical cracks will continue up to saturation of vertical cracks characterized by the full delamination of the coating from the substrate which is the final condition of coating failure.

3.2. Thick coating results

For the structural element with the coating of thickness $h_c^{(2)} = 0.6$ mm, the results in terms of damage distribution at different loading levels are reported in Fig. 3. The scenario is now quite different since beside the same mechanism of vertical cracks which form at distance length multiple pair fraction of $L_{(c)}$, inclined cracks also develops. The inclined crack instead of starting from the external surface, the are originated at the bottom and then propagates up to the surface inducing spallation of the coating. The competition in this case is among three mechanisms. Namely vertical cracks, inclined shear cracks and finally bottom delamination.

As final remark it emerges the central design concept that a greater thickness gives a better thermal coating but it has a lower mechanical resistence. Therefore the optimal thickness has to be obtained by a compromise between thermal insulation performance and mechanical resistence.

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