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Assessment of crack-related problems in layered ceramics using the finite fracture mechanics and coupled stress-energy criterion

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Abstract

This contribution gives an overview of different fracture-mechanics issues occurring in layered ceramics designed with internal compressive residual stresses (such as the edge cracking, crack arrest by the compressive layer or crack deflection/bifurcation) and proposes an effective approach to describe the initiation and/or propagation of cracks in such materials. The finite fracture mechanics (FFM) theory and the coupled stress-energy criterion (CC) are discussed and applied to understand their fracture behavior. The stress-energy coupled criterion is based on the tensile strength and toughness data of investigated material and it does not contain any adjustable parameter, which is its indisputable advantage. It could thus (in the considered brittle materials) predict both crack initiation and crack propagation under consideration of both thermal and external mechanical loading. A case study is investigated, where edge cracking in compressive layers can be predicted as a function of the thickness of the compressive layer and the magnitude of residual stresses. Another case study concerns the onset of a crack in a notched sample of a layered ceramic submitted to bending. The propagation of the crack through the ceramic laminate is studied as a function of the volume ratio of particular material components and corresponding magnitude of residual stresses in both compressive and tensile layers. Under certain combination of residual stress and layered architecture, the CC predicts crack arrest in the internal compressive layer of the laminate in accordance with experimental observations under similar loading conditions.

Keywords: Layered ceramics; crack bifurcation; edge cracking; Finite Fracture Mechanics; Coupled Criterion

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Nomenclature

a	Edge crack length (depth)
F	Loading force
G_c	Critical energy release rate, fracture energy
$G(a)$	Energy release rate as a function of edge crack length
$G_{inc}(a)$	Incremental energy release rate as a function of edge crack length
h	Crosshead displacement upon four point bend test
K_{Ic}	Fracture toughness
K_{res}	Stress intensity factor at the crack tip induced by pure residual stresses.
K_R	Apparent toughness
t_1, $t^{(ATZ)}$	Thickness of the tensile layer
t_2, $t^{(AMZ)}$	Thickness of the compressive layer
V_A, V_B	Volume of component A and B
W	Potential energy of the body
ΔT	Change of the temperature
σ_c	Critical stress – strength of material
σ_{res}	Residual stress
σ_{yy}	Normal stress along the prospective crack path

1. Introduction

Layered ceramic materials (also referred to as "ceramic laminates") have become an attractive choice for the design of structural ceramics with improved fracture toughness and mechanical reliability. The brittle fracture of monolithic ceramics has been overcome by designing layered architectures of different kind, i.e. geometry, composition of layers, residual stresses, weak interfaces, etc. The main goal of designing layered ceramics is to enhance the fracture resistance of the system and, in some cases, to decrease the sensitivity of the material strength to the defect size (i.e. increase the material flaw tolerance). The utilisation of tailored compressive residual stresses acting as physical barriers to crack propagation has succeeded in many ceramic systems – see e.g. works of Rao et al. (1999), Bermejo et al. (2007a), Bermejo et al. (2008a), Lugovy et al. (2005), Sglavo and Bertoldi (2006), Bermejo et al. (2008b). The prediction of crack initiation and propagation upon processing or external loading in such layered systems, may help to design structures without pre-existing cracks and/or with maximal fracture resistance. A limiting factor in the design of these multilayer systems is the fact that the beneficial compressive stresses in one type of layers have to be balanced by (potentially critical) tensile stresses in the counterpart layers. Therefore, the use of relatively high residual stresses to enhance the mechanical behaviour can lead to the onset of initial cracks in the layers, which may later propagate in service under external applied stresses, leading to failure of the component.

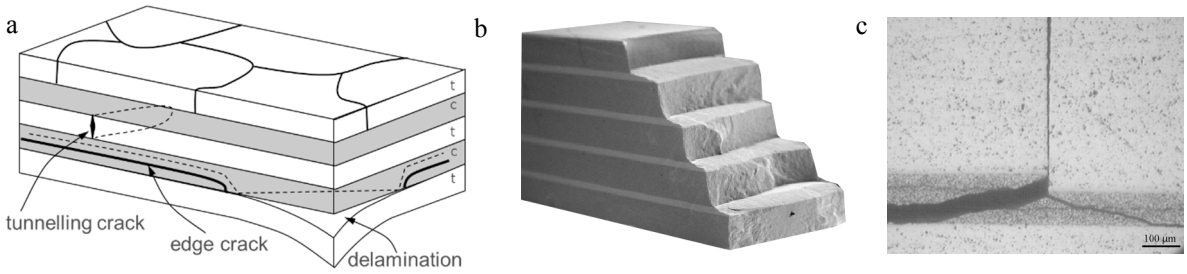

Fig. 1. (a) Schematic of surface cracks in ceramic laminates designed with tensile "t" and compressive "c" residual stresses Lube (2007), (b) Stepwise fracture of ceramic laminate with residual stresses - see Bermejo et al. (2006), (c) Detail of the crack bifurcation in compressive layer - Bermejo et al. (2007a)

Fig. 1 (a) illustrates typical cracks associated with residual stresses in planar ceramic-ceramic multilayer systems - Lube (2007). Tunnelling cracks may appear at the free surface of the layers with tensile stresses, and are oriented perpendicular to the layer plane Ho and Suo (1993), Hillman et al. (1996). Another type of cracks are the so-called "edge cracks", which initiate from pre-existing flaws at the free surface of compressive layers, oriented parallel to the layer plane Ho et al. (1995), Bermejo et al. (2006). The third type is delamination, mainly occurring at the corner interface between adjacent layers.

In this work, a 2D parametric finite element (FE) model is developed to predict the onset and propagation of both surface (edge) cracks and major cracks propagating through the ceramic laminate. The FE model utilizes the stress-energy coupled criterion (CC) - Leguillon (2002), which combines the necessary stress and energy conditions for the determination of the crack onset. Subsequent crack propagation is controlled by the Griffith criterion. Several geometries are examined, and the effect of the compressive residual stresses and thickness of the compressive layers on the fracture-mechanics behaviour of ceramic laminates is analysed.

2. Mechanical issues in layered ceramics designed with residual stresses

2.1. Edge cracking in compressive layers

Edge cracking is related to the manufacturing process of ceramic laminates with strong interfaces and relatively high compressive residual stresses. An example is shown in Fig. 2 on a multilayer architecture consisting of alternating layers of Al_2O_3-5%t-ZrO_2 (referred to as ATZ) and Al_2O_3-30%m-ZrO_2 (named as AMZ - see Bermejo et al. (2007b) for more details on the layered materials). During the cooling down process from the sintering temperature, high residual stresses (tensile/compressive) are induced in the layers (due to mismatch in coefficients of thermal expansion). At the free edge of the compressive layers, the stress redistribution develops a localized tensile stress responsible for the onset of edge cracks all along the specimen free surface – as shown in Fig. 2. The main parameters influencing this phenomenon are both the magnitude of residual compressive stress and the thickness of the compressive layer – for more details see Refs. Ševeček et al. (In press 2016), Leguillon et al. (2015b) or Chen et al. (2010).

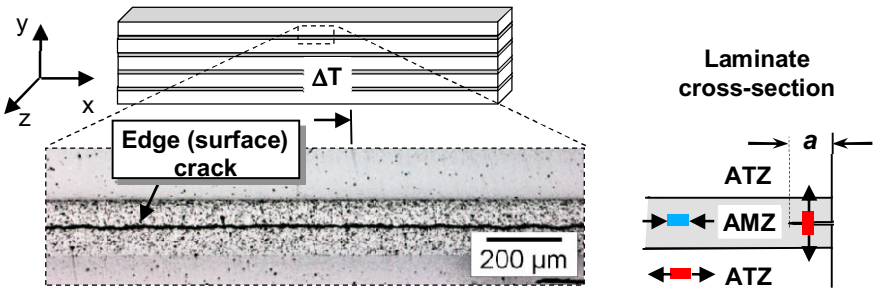

Fig. 2. Experimental observation of the edge crack phenomenon in a compressive AMZ layer, and stress redistribution at the free surface of the thin compressive layer.

2.2. Crack arrest in compressive layers

The propagation of a surface crack in a ceramic laminate may differ from the crack propagation in monolithic ceramic materials. In the later, the propagation of a surface crack upon external loading takes place in an unstable manner, i.e. when the conditions for crack propagation are fulfilled; catastrophic failure is likely to occur. However, in the former case, the propagation of an initial surface crack may not yield catastrophic fracture. In some particular cases, depending on the location and the residual stress level of the internal compressive layers, the major crack (initiated in the top tensile layer) can be arrested by the strong compressive stresses within the next layer – as shown in Fig. 3(a). To analyze such behavior a fracture mechanics analysis based on the weight function method can be employed – as shown e.g. by Sestakova et al. (2011). The apparent toughness of the laminate is calculated as a function of the crack position in the layered architecture, taking into account the contribution of the residual stresses of

corresponding layers. One can see in Fig. 3(b) that at certain depth of ATZ layer and beginning of AMZ layer the apparent toughness K_R is negative which indicates spontaneous crack propagation (even at zero external load) while in the rest of AMZ layer K_R increases rapidly, analogue to an R-curve effect. Under certain combination of compressive residual stresses, thickness and location of the compressive layer, this may lead to crack arrest – Bermejo et al. (2007b).

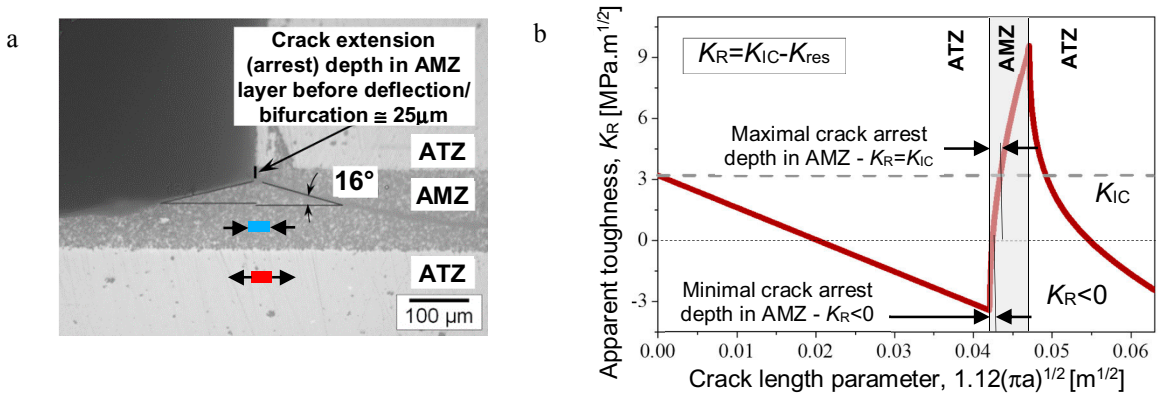

Fig. 3. (a) Experimental observation of the crack arrest in the compressive layer (before crack deflection); (b) evidence of the crack arrest based on the weight function analysis of the crack propagating through the ceramic laminate.

2.3. Increase of fracture resistance through crack deflection/bifurcation mechanisms

Laminates with strong interfaces and sufficiently high magnitudes of compressive residual stresses could exhibit a significant crack growth resistance behaviour associated with energy dissipating mechanisms such as crack deflection/bifurcation phenomena occurring during crack propagation – see Fig. 1 (b) and (c) or Fig. 3(a). The optimisation of the layered design is based on the capability of the layers to deviate the crack from straight propagation. Experimental observations have shown the tendency of a crack to propagate with an angle through the compressive layer and even cause delamination of the interface which could result in further dissipation of fracture energy. The main factor influencing presence of the crack bifurcation phenomenon are both the magnitude of the compressive residual stresses (controlled by the volume ratio of particular laminate components and by mismatch in coefficients of thermal expansion - CTE) and the thickness of the compressive layer – as shown by Leguillon et al. (2015a), Ševeček et al. (2013) and Ševeček et al. (2014). The prediction of the crack path upon loading in the layered systems will help in tailoring their design to promote a maximal resistance to fracture.

3. Finite Fracture Mechanics and coupled stress-energy criterion

An alternative approach to predict the initiation and propagation of various crack types in ceramic laminates upon thermo-mechanical loading is to employ a coupled stress-energy criterion (CC) – see works of Leguillon (2002), Leguillon et al. (2015a), Leguillon et al. (2015b). It was developed over the last decade within a more general framework of the so-called Finite Fracture Mechanics, discussed widely by authors Leguillon (2002), Martin and Leguillon (2004), Taylor et al. (2005), Cornetti et al. (2006), Cornetti et al. (2012), Yosibash (2012) and Weißgraeber et al. (2016). The CC criterion states that crack onset occurs if two necessary conditions are fulfilled simultaneously:

$$G_{inc}(a) \geq G_c \text{ and } \sigma_{yy} \geq \sigma_c. \quad (1)$$

The first condition specifies that there is enough available energy to create a crack, G_{inc} is the potential energy released by a crack per unit length, G_c is the material toughness. The second condition specifies that the tensile stress σ_{yy} is greater than the tensile strength σ_c all along the expected crack path. As a consequence of the energy balance (i.e. the first condition), the crack nucleation occurs abruptly and the crack jumps over a given length. This length is not an adjustable parameter, but a direct consequence of the two conditions: one providing a lower bound for admissible crack lengths and the other giving an upper bound. The compatibility between these two bounds is obtained

if the load is sufficiently high. The coupled criterion allows us avoiding any assumption on the existence of flaws able to trigger cracking, as is commonly used by various authors – e.g. Chen et al. (2010) and Hbaieb et al. (2007).

3.1. Edge cracking predictions

In order to illustrate the application of the stress-energy criterion to describe the edge cracking in laminates, a sample with a layered architecture is chosen (depicted in Fig. 4(a)) considering a thickness of t_2=150μm for the AMZ layers – for more details see work of Ševeček et al. (In press 2016). Since the ATZ and AMZ are strongly bonded (with strong interfaces), a tensile and compressive (in-plane) stress field is originated in the ATZ and AMZ layers, respectively (during cooling down from the sintering reference temperature).

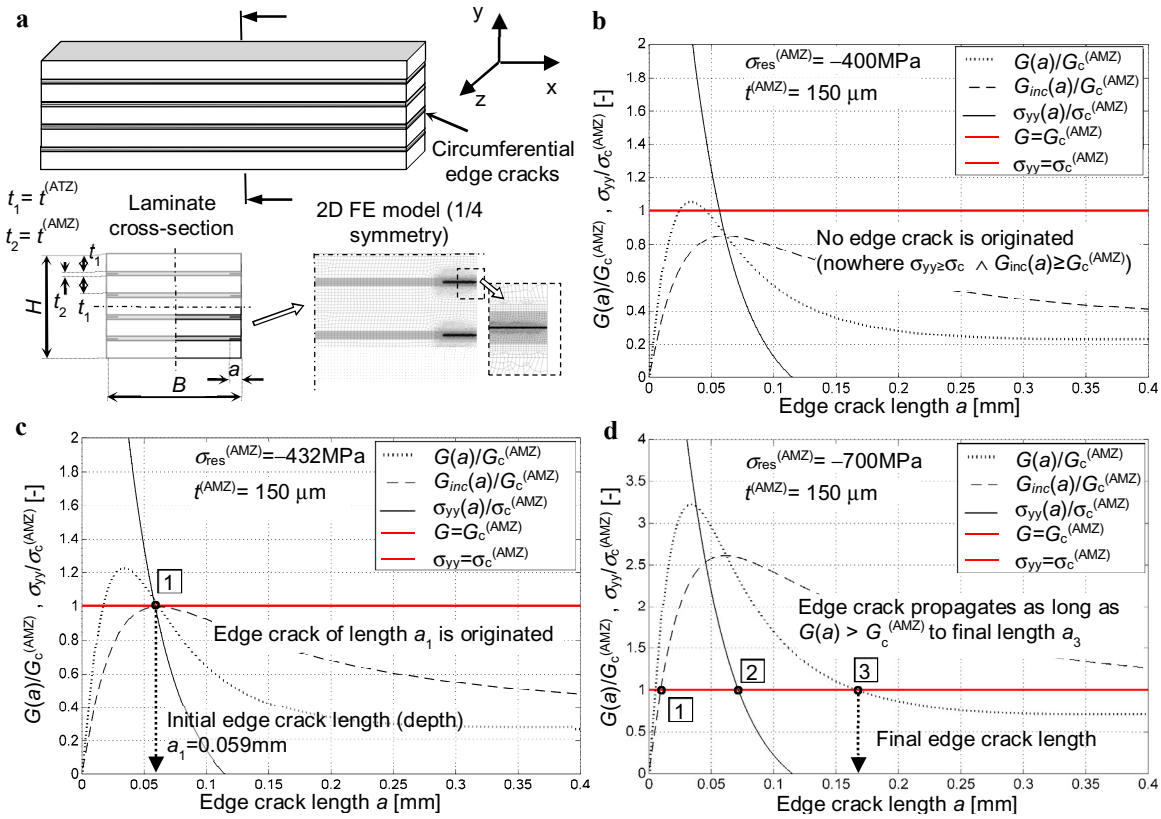

Fig. 4. (a) FE Modelling of ceramic laminate with surface (edge) cracks; (b)-(d). Application of the coupled criterion for prediction of the edge crack initiation and extension: (a) energy condition for crack initiation not fulfilled – no edge cracking, (b) both energy and stress condition is fulfilled at point 1 – edge crack of length a_1 appears

Figs. 4(b), 4(c) and 4(d) show the normalized incremental energy release rate $G_{inc}(a)/G_c^{(AMZ)}$, the normalized energy release rate $G(a)/G_c^{(AMZ)}$ and the normalized tensile stress $\sigma_{yy}(a)/\sigma_c^{(AMZ)}$ for a given AMZ layer thickness, i.e. $t^{(AMZ)}$ = 150 μm, and compressive residual stresses (in the AMZ layers) of –400 MPa, –432 MPa, and –700 MPa, respectively (corresponding to ΔT values of –730 °C, –788 °C and –1280 °C, respectively). In case of Fig. 4(b) no edge cracking is possible, because the energy condition is not fulfilled at any point. In Fig. 4(c) both criteria are fulfilled at point 1 and edge crack is thus originated and with increasing residual stress (as shown in Fig. 4(d)) edge crack follows Griffith´s criterion and propagates as long as $G(a) > G_c^{(AMZ)}$.

The critical thickness of the AMZ layer leading to the edge cracking, i.e. $t_c^{(AMZ)}$, can also be described using the equation derived (in a similar form) by Ho et al. (1995) and employed also by Chen et al. (2010):

$$t_c^{(\mathrm{AMZ})} = \frac{K_{Ic}^{2\ (\mathrm{AMZ})}}{C \cdot \sigma_{\mathrm{res}}^{2\ (\mathrm{AMZ})}}, \tag{2}$$

where K_{Ic} is the fracture toughness of the compressive layer, σ_{res} the in-plane compressive residual stress and C is a constant as estimated by the above authors to be equal to 0.34. By implementing the CC approach to the solution of the edge cracking problem and fitting of results by Eq. (2), we obtain a very similar result for C constant – namely C=0.32 and very good agreement of this relation with predictions made by the CC, especially in the region of residual stresses −700MPa to −350MPa - Ševeček et al. (In press 2016). Nevertheless, for residual stresses higher than −350MPa, Eq. (2) may no longer be valid, and thus predictions made by the CC should be taken into account preferably. In layers with thickness above the $t_c^{(\mathrm{AMZ})}$ an edge crack of certain depth is always originated and if the thickness or residual stress overcome another critical level, the edge crack could even grow through the entire layer and lead to its total fracture. Parametric study, relating the final edge crack depth to thickness of the compressive layer and the corresponding magnitude of residual stress is also presented in the referred paper.

3.2. Crack propagation through a ceramic laminate

A second group of fracture-mechanics issues in ceramic laminates concerns the crack propagation through the layers (originated e.g. at a prepared notch or at a surface defect) subjected to an external mechanical load. Such fracture process starts, for instance, with the crack initiation at the tip of the sharp/rounded notch, then the crack jumps up to the beginning of the next compressive layer, where it is usually arrested (due to compressive residual stresses) and additional load is required for its further propagation – see particular stages in Fig. 5. When the critical level of external load is reached, the crack starts to propagate again, nevertheless in a strongly deflected direction (again due to compressive stresses). Under certain conditions (discussed in work of Leguillon et al. (2015a) or Ševeček et al. (2013)) also crack bifurcation may occur. The crack propagation continues further until the crack reaches the next interface with tensile layer and interface delamination follows. After the delamination crack reaches certain length, it kinks out from the interface into the next tensile layer and such propagation continues until the total fracture of the specimen.

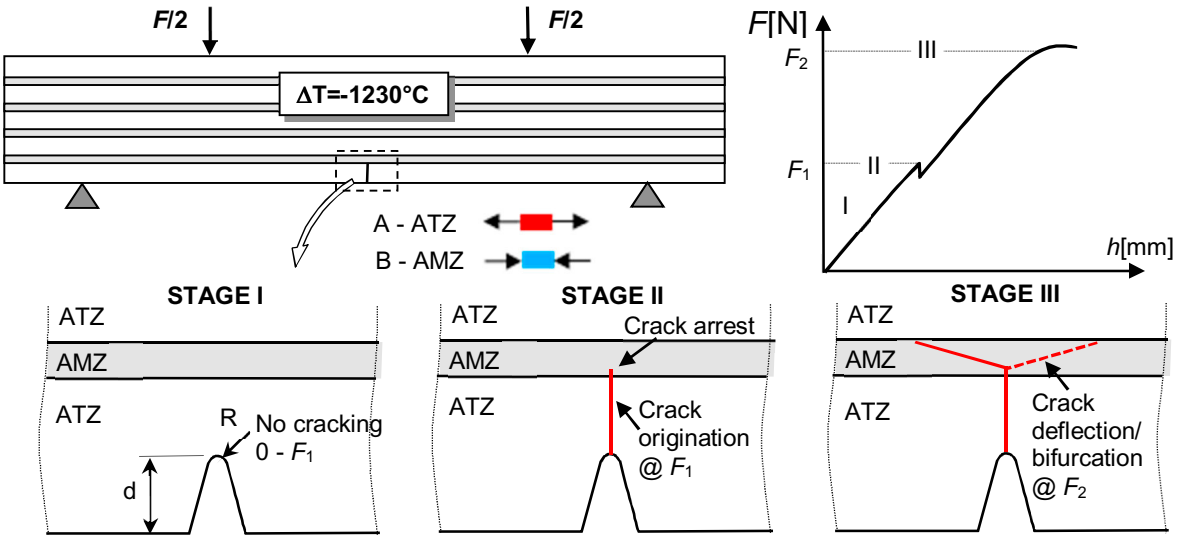

Fig. 5. Usual stages of the crack propagation in notched ceramic laminate specimen upon the 4 point bending test (applied force F).

Stage II and III can be predicted using again using CC – as demonstrated in Fig. 6. Crack initiation at a (rounded) notch and crack arrest in the AMZ layer (stage II in Fig. 5) is predicted by corresponding dimensionless stresses and energy release rates plotted in Fig. 6(a).This plot shows critical conditions in the laminate under applied force F_1=42N (and taking into account also residual stresses after laminate processing) necessary to initiate a crack at a rounded

notch of depth d=180μm. This state is indicated by simultaneous satisfaction of stress and energy condition ahead the notch tip ($\sigma_{yy}/\sigma_c=G_{inc}/G_c=1$) – indicated by point 1. Once the crack is initiated it follows Griffith criterion (dash-and-dotted line) and propagates until K_I at the crack tip is higher than K_{Ic} or at the most $K_I=0$ - indicated by point 2 (corresponding to crack arrest in AMZ layer) – for more details see work of Leguillon et al. (2015a) and Ševeček et al. (2013). Finally the Fig. 6(b) shows predictions of crack bifurcation/deflection starting usually at the arresting point 2 after reaching of critical force F_2 (see Fig. 5). The crack will propagate in direction where change of potential energy δW (induced by creation of new crack surfaces) reaches its maximal value. One can thus distinguish also between single crack deflection and crack bifurcation - for more details see Leguillon et al. (2015a) and Ševeček et al. (2013).

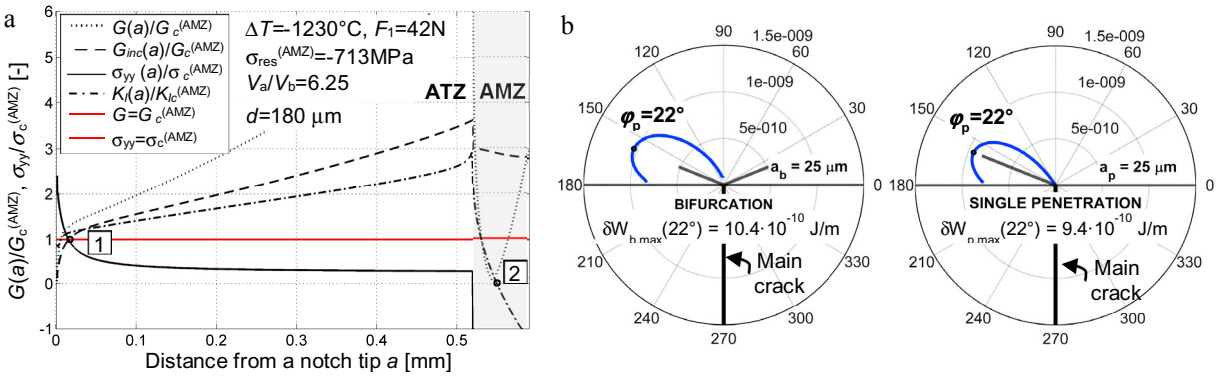

Fig. 6. (a) Crack propagation from a rounded notch and crack arrest in the AMZ layer, (b) crack bifurcation prediction based upon values of change of the potential energy in various admissible propagation directions.

4. Outlook

Additional work is needed to validate the obtained results on different real specimens with various thicknesses and levels of residual stresses, aiming to provide guidelines for the fabrication of layered ceramics with controlled surface cracks. The proposed approach, based on FFM and coupled criterion will be further applied on systems combining brittle and ductile materials (e.g. ceramics and metals) to investigate crack initiation and extension within the brittle component. Predictions will be verified by experiments and if both will provide sufficient agreement the CC is intended to be employed for fracture-mechanics assessment of structural components with metallic phase which are now of high point of interest, especially for lifetime assessment of various electronic devices - Bermejo et al. (2011).

5. Conclusions

This work presents a novel approach to predict the onset and propagation of various types of cracks in ceramic laminates containing high residual stresses (e.g. edge cracks and cracks propagating through the laminate). A fully parametric 2D FE model has been developed to simulate the initiation and propagation of such cracks within a multilayer structure. The conditions for crack initiation/propagation are assessed using a stress-energy coupled criterion outgoing from the FFM theory. The analysis only requires the values of the elastic modulus and Poisson's ratio of the layers, the coefficient of thermal expansion, and the toughness and tensile strength of the tensile/compressive layer. There is no adjustable parameter, and there is no need to assume the presence of surface defects to initiate fracture. Based upon the presented model, recommendations on layer architectural design preventing e.g. the formation of edge cracking or leading to increased apparent fracture toughness of such systems can be given and may open new possibilities in the design of multilayer structures with enhanced mechanical properties. Suggested technique of CC exhibit also a good agreement with experimental observations.

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