Estimation of stepwise crack propagation in ceramic laminates with strong interfaces

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ABSTRACT. During the last years many researchers put so much effort to design layered structures combining different materials in order to improve low fracture toughness and mechanical reliability of the ceramics. It has been proven, that an effective way is to create layered ceramics with strongly bonded interfaces. After the cooling process from the sintering temperature, due to the different coefficients of thermal expansion of individual constituents of the composite, significant internal residual stresses are developed within the layers. These stresses can change the crack behaviour. This results to the higher value of so-called apparent fracture toughness, i.e. higher resistance of the ceramic laminate to the crack propagation. The contribution deals with a description of the specific crack behaviour in the layered alumina-zirconia ceramic laminate. The main aim is to clarify crack behaviour in the compressive layer and provide computational tools for estimation of crack behaviour in the field of strong residual stresses. The crack propagation was investigated on the basis of linear elastic fracture mechanics. Fracture parameters were computed numerically and by author's routines. Finite element models were developed in order to obtain a stress distribution in the laminate containing a crack and to simulate crack propagation. The sharp change of the crack propagation direction was estimated using Sih's criterion based on the strain energy density factor. Estimated crack behaviour is qualitatively in a good agreement with experimental observations. Presented approach contributes to the better understanding of the toughening mechanism of ceramic laminates and can be advantageously used for design of new layered ceramic composites and for better prediction of their failure.

KEYWORDS. Ceramic laminates; Crack behaviour; Residual stresses; Strain energy density factor; Crack propagation direction.

INTRODUCTION

Material interfaces play an important role in material (composite) behaviour and its properties. The presence of regions with different material and mechanical properties and the existence of an interface between them have a pronounced influence on the stress distribution of composite bodies. The influence of material interfaces was intensively studied during last years for different material combinations, from both theoretical and experimental sides, see e.g. [1-8] for detailed information. The specific stress distribution of layered composites can be used in design of new composite materials with improved mechanical properties, e.g. with higher flexural strength or higher resistance to crack propagation, etc. The existence of interfaces and their toughening effect are, with the advantage, used in the manufacturing of "flaw tolerant" multilayer ceramic composites [9]. There is a new class of ceramic materials under development, the ceramic laminates with controlled crack resistance and crack propagation [10-12]. The paper is focused on ceramic laminates with strongly bonded layers. The toughening mechanism of strongly bonded laminates is based on deflection and/or bifurcation of crack path caused by internal residual stresses inside the layers [13,14]. Mechanism of internal stresses evolution is based on unequal shrinkage of physically bonded materials during sintering [15]. This mechanism was experimentally proved for different kinds of ceramic laminates with strongly bonded interfaces [16-27], however only few works exists dealing with the prediction of laminate properties [28] or explaining specific crack behaviour in the ceramic laminates [29-32]. This paper focuses on the crack behaviour in the compressive layer of the laminate and describes by use of linear elastic fracture mechanics specific crack propagation (see Fig. 1) in this layer.

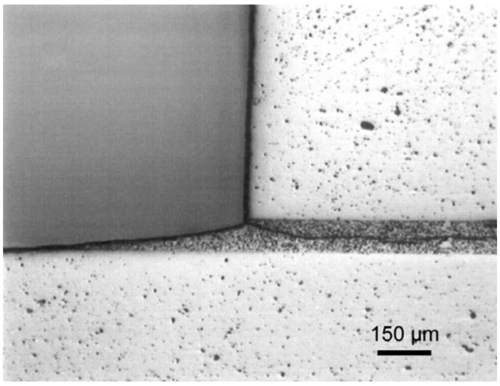


Figure 1: Crack bifurcation in AMZ layer. With courtesy of R. Bermejo [23].

The basic principle of the toughening of the layered ceramic composite is based on selection of two ceramics with different values of coefficients of thermal expansion. The ceramics are layered by system A-B-A symmetrically and parallelly to the axis of symmetry of the layered composite body. Cooling down from the sintering temperature leads to the development of residual stresses, which are usually of tensile nature in the outside layers.

Description of the studied layered ceramic composite

For the study material system based on alumina and zirconia was chosen. These two constituents can be taken as typical examples of convenient materials for layered ceramics. Behaviour of such kind of laminates were studied e.g. in [20-23]. Considered ceramic laminate was created by 9 layers. 5 were made of Al_2O_3/5vol.%t-ZrO_2 (alumina with tetragonal zirconia, reffered as ATZ) and 4 were made of Al_2O_3/30vol.%m-ZrO_2 (alumina with monoclinic zirconia, reffered as AMZ). Material characteristics were taken from literature [20,21] and are summarized in Tab. 1. The laminate was subjected to four-point bending (4PB) test, see Fig. 2.

Property	ATZ	AMZ
Young´s modulus E [GPa]	390	280
Poisson´s ratio ν [-]	0.22	0.22
Fracture toughness K_{IC} [MPa.m$^{0.5}$]	3.2	2.6
Coefficient of thermal expansion α_t [$10^{-6}K^{-1}$]	9.8	8.0
Strength σ_f [MPa]	422	90

Table 1: Material properties of studied laminate [20,21].

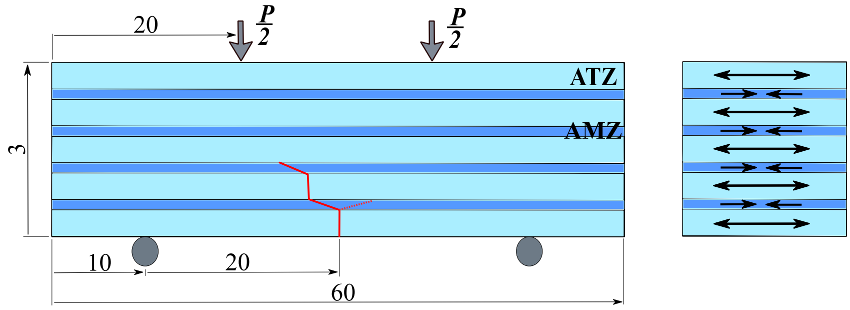


Figure 2: Scheme of studied ceramic laminate with typical crack path (dimensions in [mm]) and orientation of residual stresses in composite layers.

The magnitude of residual stresses in the case of crack absence in the layered composite can be estimated from forces balance in individual layers. This leads to following expressions [33]:

$$\sigma_{res,ATZ} = \frac{\int_{T_{sf}}^{T_0} (\alpha_{AMZ} - \alpha_{ATZ}) dT}{\frac{1}{E'_{ATZ}} + \frac{1}{E'_{AMZ}} \cdot \rho \cdot \frac{N+1}{N-1}}, \qquad \sigma_{res,AMZ} = -\sigma_{res,ATZ} \cdot \rho \cdot \frac{N+1}{N-1}, \tag{1}$$

where: $\rho = \frac{t_{ATZ}}{t_{AMZ}}$, $E'_{AMZ} = \frac{E_{AMZ}}{1-\nu_{AMZ}}$, $E'_{ATZ} = \frac{E_{ATZ}}{1-\nu_{ATZ}}$, T_{sf} [°C] is stress free temperature, T_0 [°C] room temperature, α [10^{-6}K^{-1}] coefficient of thermal expansion, N [-] number of layers, t [mm] thickness of layer, E [MPa] Young´s modulus and ν [-] Poisson´s ratio. Calculated values of residual stresses for studied configurations are shown in the Tab. 2.

$t_{ATZ} : t_{AMZ}$	t_{ATZ} [mm]	t_{AMZ} [mm]	$\sigma_{res,ATZ}$ [MPa]	$\sigma_{res,AMZ}$ [MPa]
2 : 1	0.4288	0.2140	236.6	-592.6
5 : 1	0.5170	0.1038	109.8	-683.6
7 : 1	0.5384	0.0770	80.6	-704.6
10 : 1	0.5556	0.0556	57.7	-721.0

Table 2: Residual stresses calculated for different ratio of layer thicknesses ($t_{ATZ} : t_{AMZ}$) by Eq. 1.

It is evident from the Tab. 2 that the compressive residual stresses in the AMZ layers are circa six hundred megapascals and higher for all considered cases. These stresses are responsible for typical stepwise crack propagation like is shown in the scheme in Fig. 2.

MODEL OF CRACK PROPAGATION

Estimation of crack propagation direction

Sih´s criterion [34,35] based on strain energy density factor S was used for the determination of crack propagation direction due to brittle nature of the composite. The criterion was implemented in finite element system Ansys [36] to perform calculations with small crack increments automatically:

$$S = a_{11}K_I^2 + 2a_{12}K_I K_{II} + a_{22}K_{II}^2, \tag{2}$$

where K_I and K_{II} are stress intensity factors corresponding to mode I and II respectively,

$$a_{11} = \frac{1}{16\mu}\left[\left(1+\cos\theta\right)\left(k-\cos\theta\right)\right],$$
$$a_{12} = \frac{1}{16\mu}\sin\theta\left[2\cos\theta-\left(k-1\right)\right],$$
$$a_{22} = \frac{1}{16\mu}\left[\left(k-1\right)\left(1-\cos\theta\right)+\left(1+\cos\theta\right)\left(3\cos\theta-1\right)\right],$$

constant $k = 3-4\nu$ for plane strain or $k = \frac{3-\nu}{1+\nu}$ for plane stress, $\mu = \frac{E}{2\left(1+\nu\right)}$ is shear modulus, θ is polar coordinate originating from the crack tip.

The criterion postulates that the crack will propagate in the direction where factor S is the minimum. The angle of next crack propagation direction θ_0 can be determined from the conditions:

$$\left(\frac{\partial S}{\partial\theta}\right)_{\theta=\theta_0} = 0 \wedge \left(\frac{\partial^2 S}{\partial\theta^2}\right)_{\theta=\theta_0} > 0 \tag{3}$$

The crack will propagate under angle θ_0 if the value of S will reach its critical value S_{cr}, i.e. for $S = S_{cr}$. In special case (pure mode I) can be the critical value S_{cr} related to fracture toughness K_{Ic}:

$$S_{cr} = \frac{\left(1-2\nu\right)K_{IC}^2}{4\mu} \quad \text{for plane strain condition.} \tag{4}$$

Fracture toughness of AMZ layer is 2.6 MPa.m$^{0.5}$. Corresponding value of S_{cr} = 825.10^{-8} MPa.m.

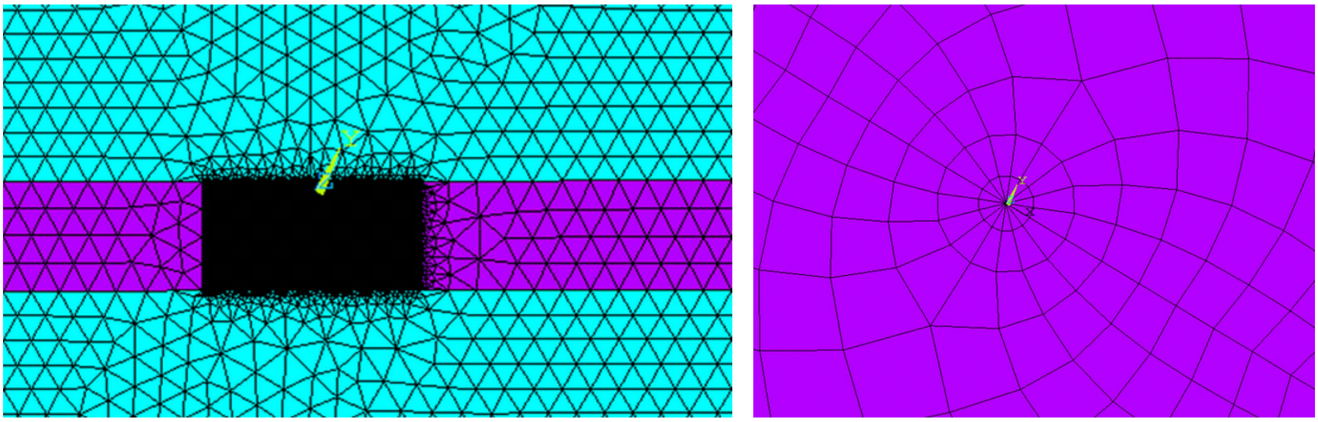


Figure 3: Detail of fine mesh around the crack tip.

Numerical model

For the numerical modelling finite element (FE) method was chosen. Numerical models were developed in commercial system Ansys. Models contained circa 100 000 elements PLANE 183. Boundary conditions corresponding to 4PB, i.e. vertical displacements on the lower side in the locations of rigid supports were equal to zero and the loading forces $P/2$ on the upper side of the models were applied, see Fig. 2 for details. Thermal load by change of temperature from 1200°C to 20°C was applied together with mechanical loading to generate residual stresses in the layers. Material characteristics written in the Tab. 1 were used. All calculations were performed under condition of plane strain. Very fine mesh was used around the crack tip to well describe the stress distribution there (see Fig. 3), which is of crucial importance for determination of crack behavior. The size of smallest elements was circa 1.10^{-5} mm. On the base of former experience [28] the crack propagation was modelled from first ATZ/AMZ interface through the AMZ layer. The initial crack increment was chosen 1 μm to describe crack path precisely and model was remeshed after each step. Stress intensity factors were calculated by author's routine from displacements close to the crack tip in each step. New crack propagation direction was determined on the base of author´s Ansys macros based on Eqs. 2 and 3 after each step. Hundreds of calculations were performed to obtained realistic crack path in compressive AMZ layer during each simulation. PC based workstations were used for extensive numerical calculations.

RESULTS AND DISCUSSION

Different material layers create regions with different material properties. It was shown in the former work of authors [7] that suitable selection of materials with different elastic properties can lead to the higher values of applied load for crack propagation through interface. This value of applied load can be higher than the one for crack propagation in the individual composite constituents. The effect of crack retardation is stronger in the studied case due to acting of residual stresses developed in the layers during sintering process. These residual stresses have pronounced influence on the crack behaviour in the composite, damage mechanism of the composite and consequently on the value of apparent fracture toughness of the composite body.
In the numerical FE studies four different ratios of layer thicknesses were considered (see Tab. 2). The calculations performed were focused on the description of mechanism leading to the higher apparent fracture toughness of ceramic laminate with strongly bonded interfaces. Sih's criterion (Eq. 3) was applied in each step of the simulations. The crack started to strongly deflect in certain depth *a´* under the first ATZ/AMZ interface due to acting of compressive stresses in all simulations. In this moment an additional external load was necessary for the crack propagation. The depth of deflection and values of external force *P* are shown in the Tab. 3.

$t_{ATZ} : t_{AMZ}$	a' [mm]	P_{max} [N]
2 :1	0.046	16.2
5 : 1	0.020	24.8
7 : 1	0.017	34.6
10 : 1	0.024	48.0

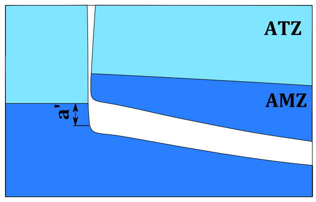
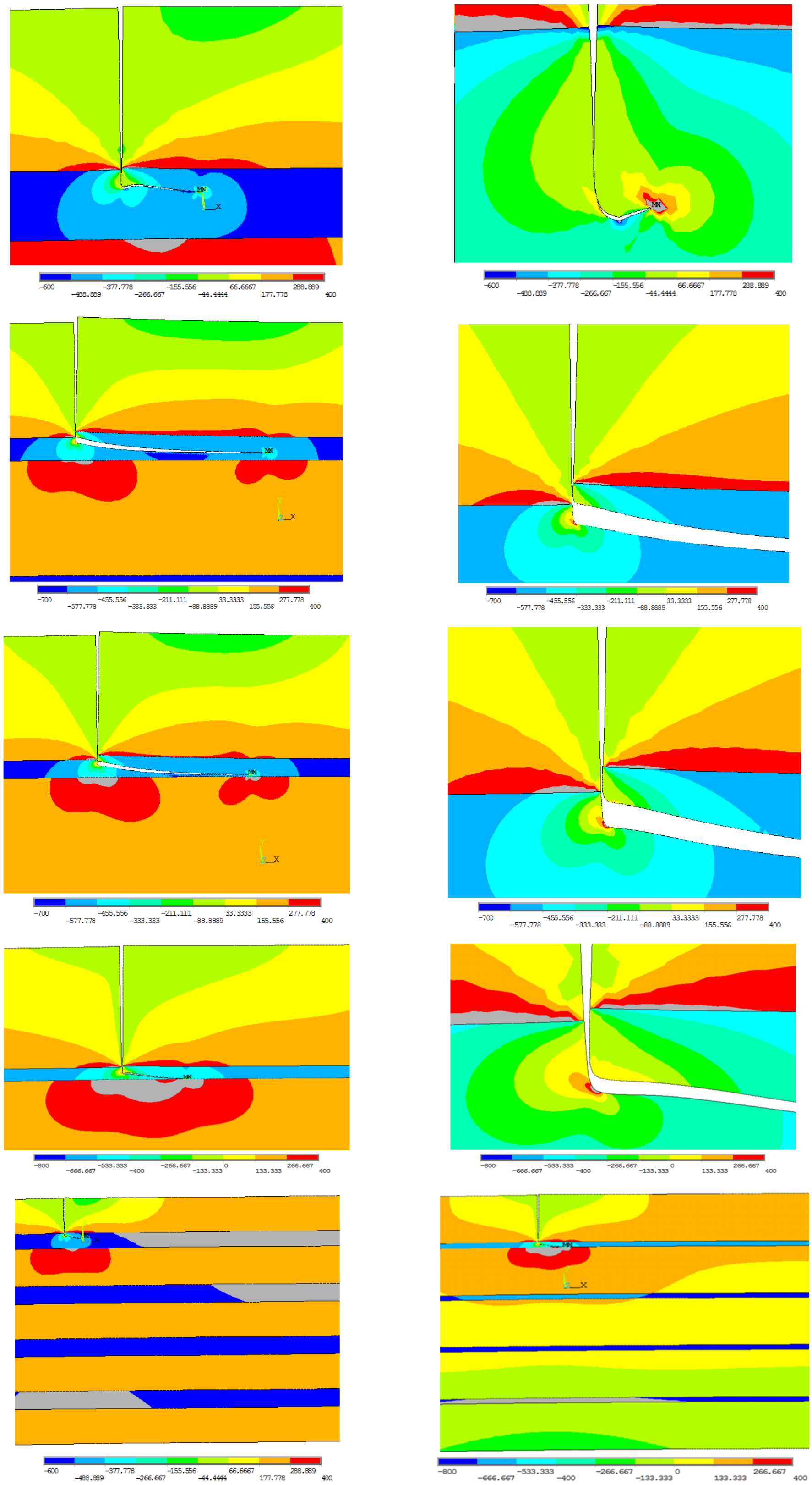


Table 3: The depth *a´* in AMZ layer under the first ATZ/AMZ interface, where the crack changes mode of propagation and values of the force *P* acting in the moment of crack deflection.

Hundreds of calculations (steps) were performed in each simulation to obtain crack path in the AMZ layer. Results of simulations are shown in the Fig. 4.
On the base of results obtained the crack behaviour in the compressive layer can be divided to four stages, see Fig. 5 for the explanation:

1) After passing perpendicularly through the ATZ/AMZ interface the crack is retarded (the stress intensity factor and the strain energy density factors decrease). An external load is necessary for further crack propagation. The compressive stresses don't allow further direct crack propagation under mode I like in tensile loaded ATZ layer.
2) In the depth *a´* under the interface the character (mode) of crack propagation changes from mode I to mode II. The stress distribution around the crack tip in the depth *a´* enables crack deflection or bifurcation. Further crack propagation is controlled by compressive stresses. The crack propagates parallel or nearly parallel to the material interfaces.
3) When the crack tip is close to the next AMZ/ATZ interface the presence of tensile stresses in the ATZ layer growths in importance and the controlling mode of crack propagation starts to be again mode I and the crack deflect to the direction (nearly) perpendicular to AMZ/ATZ interface.
4) The crack passing through (nearly) perpendicularly the AMZ/ATZ interface. The resistance to the crack propagation is the highest between stages 3 and 4. Behaviour of the crack at the stage 4 was studied in [28].



a) Result for t_{ATZ} : t_{AMZ} = 2. Crack path in the AMZ layer after 270 steps (left), detail of crack deflection after 33 steps.

b) Result for t_{ATZ} : t_{AMZ} = 5. Crack path in the AMZ layer after 491 steps (left), detail of crack deflection.

c) Result for t_{ATZ} : t_{AMZ} = 7. Crack path in the AMZ layer after 315 steps (left), detail of crack deflection.

d) Result for t_{ATZ} : t_{AMZ} = 10. Crack path in the AMZ layer after 306 steps (left), detail of crack deflection.

e) Detail of stress distribution in the laminates: t_{ATZ} : t_{AMZ} = 2 (left), t_{ATZ} : t_{AMZ} = 10.

Figure 4: Simulation of crack propagation in the compressive layer for different ratio of layer thicknesses. Magnitude of longitudinal stress component is displayed.

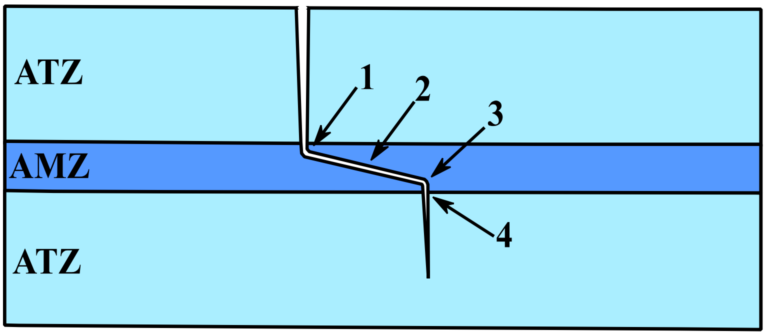


Figure 5: Scheme of stages of crack propagation in the compressive layer of ceramic laminate with strongly bonded interfaces.

The crack can relatively easy propagate in the outside layers from some flaws, scratches or initial notches under external bending load of the composite. In the tensile layers the crack propagation corresponds to the mode I and cracks propagate perpendicularly to the material interface. Due to this fact it is necessary to prepare the composite with low tensile stresses, i.e. with wide tensile layer (ATZ in studied case) and thin compressive layer (AMZ) with high compressive stresses. The resistance to the crack propagation in the tensile layer is lower due to tensile residual stresses than in the case of crack propagation in the homogeneous ceramics, see e.g. [28]. When the crack passed through the interface to the compressive layer (AMZ) acting compressive residual stresses change the mode of crack propagation from mode I to shear mode II. This causes strong crack deflection or can lead to bifurcation of the propagating crack. Crack propagation parallel to the material interface in the compressive layer is evident from experiments published in [37]. This phenomenon is supported by results obtained as well. The parallel crack propagation is controlled by specific stress distribution in the compressive AMZ layer and influenced by the vicinity of tensile layers. After some propagation the bending nature of loading, existence of material imperfections (flaws, pores) and the vicinity of material interface lead to the other change of crack propagation direction close to AMZ/ATZ interface [32]. These effects contribute to the characteristic stepwise crack propagation in the strongly bonded ceramic laminates.

CONCLUSIONS

The paper presented focuses on the crack behaviour in the multilayered ceramic composite subjected to the bending load. Crack propagation in the compressive layer responsible for higher apparent fracture toughness of the composite was investigated by means of finite element method. Sih's criterion based on strain energy density factor was used for estimation of the crack behaviour in the layers and for the estimation of crack path. It was shown that the crack after passing through the first material interface between tensile and compressive layer retards due to acting of strong residual stresses and the crack is sharply deflected. An additional external load is necessary for further crack propagation at this moment. The depth of crack deflection was determined for different thicknesses of the composite layers. The stress distribution allows in this moment bifurcation of the crack as well, like was shown e.g. in the works [29,31]. Further crack propagation in the compressive layer is more or less parallel to the material interface. The stages leading to the stepwise crack propagation were described in detail. Finite element method implemented in commercial system Ansys with author's routines was used for numerical simulations.
The paper contributes to the better understanding of damage of strongly bonded ceramic laminates and their toughening mechanism.

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