Application of damage models to the ductile-brittle transition region of Reactor steels

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Abstract Two German ferritic pressure vessel steels (JFL, JQR) are examined in the brittle to ductile transition regime as function of temperature and irradiation. The experiments are done by a miniaturized Small-Punch-Test (SPT) in hot cells within the temperature range of -185°C up to 70°C.
From the load-displacement curve of the SPT, the yield curves and parameters of both a non-local GURSON-TVERGAARD-NEEDLEMAN ductile damage model and the BEREMIN-model are identified. The influence of temperature and irradiation on the determined model parameters is analyzed. All parameters are verified by comparison with results from standard test methods.
The parameters, identified from SPT, are used to simulate the failure behaviour in standard fracture mechanics specimens. In the upper shelf, the non-local GTN-model is applied to simulate J-Δa-resistance curves, from where the fracture toughness data J_{Ic} could be successfully predicted. In the lower shelf, the WEIBULL-stress of the specimens was computed to find out the statistics of K_{Ic} - values. Finally, a modified BEREMIN-model and the non-local GTN-model were combined to evaluate the failure of fracture specimens in the brittle-ductile transition region. This way, an acceptable agreement with Master-curve data for non-irradiated steels could be achieved over the whole temperature range.

Keywords non-local GTN-model, Beremin-Model, small-punch-test, brittle-ductile transition

1. Introduction

The quantification of irradiation effects on ferritic steels is an essential task to warrant the safety of existing nuclear power plants. While a large number of tests is needed for the description of the brittle and transition region, the available volume of irradiated material for testing is very limited.
Damage mechanics can be used to assess the integrity of mechanical structures with micro-defects through the evaluation of local criteria. In contrast to the methods of linear-elastic and elastic-plastic fracture mechanics, this approach, the concept of the Local Approach [1], can in principle be applaied to any structure. The application of the Local Approach to determine fracture mechanical properties requires the exact knowledge of the hardening and softening behavior of the material.
A promising method for the description of the failure behavior of ferritic steels in the brittle, transition and ductile region consists in minimal invasive sampling and testing of miniaturized specimens followed by the numerical simulation of standard fracture mechanical tests to predict fracture mechanical properties.
The small punch test (SPT, [2]-[6]) is a miniaturized deep drawing process that requires only tiny volumes of material. Its load displacement curve contains information about the elastic, hardening and softening properties of the tested material.
Cleavage fracture is the typical failure mechanism observed when testing in the brittle and transition region. The probability of cleavage fracture depends on the distribution of microcracks resulting from microplastic deformation, which causes a large scatter of the fracture mechanical properties. Therefore, a probabilistic model such as the Beremin local approach model [7][8], is required to

describe the failure in the brittle or transition region. It quantifies the probability of cleavage fracture based on the weakest link theory and the Griffith criterion.

Due to the absence of an initial macroscopic crack and a rather small stress triaxiality compared to fracture mechanic specimens, large parts of the SPT specimen undergo high plastic deformations even if brittle fracture is finally observed. In any case, the evolution of ductile damage precedes failure. Therefore, it is necessary to account for the influence of ductile damage when identifying material properties from the measured load displacement curves of the SPT.

In this paper, fracture toughness values are predicted solely by numerical simulation of fracture mechanics tests using material parameters identified from the SPT. A non-local formulation of a ductile damage model is used in combination with a modified Beremin model to characterize the fracture behavior of pressure vessel steels in the transition region.

2. Damage models

2.1. Non-local ductile damage model

When standard continuum damage models are implemented numerically using the finite element method, they exhibit a high sensitivity of the results to the spatial discretization size [9][10]. Material softening due to the evolution of damage localizes in a small portion of the model that is controlled by the finite element mesh, i.e. the finite element size becomes an additional model parameter. As a consequence, it is generally not possible to use the same damage model parameters in dissimilar FE models with very different element sizes.

A common idea of different methods to reduce the mesh sensitivity of damage models is to account for the influence of the surrounding material at a given material point in the constitutive equations. This results in a formulation that introduces a characteristic length scale into the model. Non-local formulations [11][12] of damage models may be divided in to three main types: formulations of the integral type, explicit gradient formulations and implicit gradient models.

The continuum damage model established by Gurson and modified by Tvergaard and Needleman (GTN, [13]-[15]) provides the basis for the constitutive equations applied in the present work. It was developed to describe the growth and coalescence of initially present or later nucleating voids in isotropic ductile materials. The GTN model accounts for the growth, nucleation and coalescence of voids. It consists of the yield condition and evolution equation for the two relevant internal variables. The change of the void volume fraction is determined by the growth of existing voids and the nucleation of voids in the matrix.

Motivated by the approach of generalized continua, the GTN continuum damage model is modified by replacing the dilatational part of the plastic strain rate by its non-local spatial average in the evolution equation for the growth of existing voids.

$$\dot{f}_G^{nl} = (1 - f)\,\dot{\bar{\varepsilon}}_p$$

All other equations of the GTN model remain untouched. For the considered case of elastic strains being small compared to plastic strains, the change of the micro-volume becomes an additional degree of freedom. The local behavior is sustained for the elastic case. The non-local dilatational part of the plastic strain rate is treated as an additional independent field quantity that is governed by the partial differential equation of the Helmholtz type

$$\overline{\varepsilon}_p - c\nabla^2\overline{\varepsilon}_p = \varepsilon_p \ ,$$

where the local hydrostatic part of the plastic strain rate ε_p acts as a source term. The constant c can be regarded as an internal length parameter that controls the influence of the surrounding material. To complete the implicit gradient formulation, homogeneous Neumann boundary conditions are chosen at all boundaries to solve the averaging equation. Details of the non-local damage model and its numerical implementation into the commercial FEM software ABAQUS can be found in [16].

2.2. Modified Beremin-Model

In the transition region both ductile damage and brittle fracture occur. Therefore, material models are needed that represent both micromechanical processes independently. The combined use of a non-local GTN-model together with the Beremin model for the calculation of the probability of cleavage fracture is conceivable in principle. However, the problems that accompany the original Beremin are getting worse when ductile damage is considered, i.e. dependence of the Weibull parameters with regard to sample shape, temperature and strain rate, difficulties in the iterative determination of the Weibull parameters, and large variations in the calculated probabilities of cleavage fracture.

Bordet et al [17] discussed that the above problems are a result of a oversimplified description of local cleavage in the Beremin model. Already in [7], a proposal for the consideration of the influence of plastic strain is made. Further modifications of the Beremin model, mainly concerning the calculation of the Weibull stress can be found in [18]-[23].

In this paper, we apply a modification proposed by Bernauer et al [24]. This modification takes into account that the nucleation of voids is promoted by the presence of carbide particles, either by the detaching of the surrounding matrix or the breaking of the particles. Both lead to the formation of cavities, whereby the initiation of cleavage fracture is no longer possible at this point. Therefore, the number of active micro-cracks is variable in the modification proposed by Bernauer. The modified Weibull stress is calculated numerically as

$$\sigma_W^B(t) = \sqrt[m]{\sum_{i=1}^{N_{pl}} \frac{V_i}{V_0} \cdot \max_{\tau \le t}\left\{\sigma_{B_1} + \sigma_{B_2}\right\}}$$

with

$$\sigma_{B_1} = \left(\sigma_I^i(\tau)\right)^m \cdot \left(1 - \frac{c_n}{f_n}\sum_{t_j \le \tau} f_N^i\left(\Delta t_j\right)\right)$$

$$\sigma_{B_2} = \sum_{t_j \le \tau}\left(\left(\sigma_I^i\left(t_j - 1\right)\right)^m \cdot \frac{c_n}{f_n} f_N^i\left(\Delta t_j\right)\right) .$$

As in the original model, the probability of cleavage fracture is determined according to

$$P_f(L) = 1 - \exp\left\{-\left(\frac{\sigma_W(L)}{\sigma_u}\right)^m\right\} .$$

In conjunction with the non-local ductile damage model, the nucleation of voids and the associated reduction of cleavage initiation points can be considered.

3. Identification of material properties

For a small initial void volume fraction of the investigated material ductile damage affects the behavior of the SPT specimen in a deformation state, where large equivalent plastic strains occur. Accordingly, the parameter identification is performed in two phases: First, the yield curve parameters are determined neglecting ductile damage. Here, the material is modeled as elastic-plastic with the von Mises yield condition and the associated flow rule with isotropic hardening. Subsequently, the identification of the ductile damage parameter is carried out together with the adoption of a reduced number of yield curve parameters.

3.1. Identification of yield curves

For the determination of yield curves from measured load-displacement curves of the SPT, a method was used, which does not require FEM calculations during the identification process. Instead, previously trained Neural Networks are used. The parameter determination is done by minimizing the difference between measured load-displacement curves and those approximated by the Neural Networks. The optimization algorithm simulated annealing (SA, [25]) was used. Details of the identification of yield curves can be found in [4].

3.2. Identification of the parameters of the non-local ductile damage model

The identification of damage parameters is done after the determination of the yield curve parameters, now with ductile damage taken into account. Here, the parallel optimization algorithms Appspack and Hopspack are used [26]-[28] . Both algorithms are based on Generating Set Search Methods (GSS, [29][30]), a class of derivative-free optimization methods. The asynchronous parallel implementations Appspack and Hopspack start FE-simulations on different processors; the algorithms are not waiting for the results of simultaneous calculations.

3.3. Identification of Weibull-parameters

For the determination of the Weibull parameters load-displacement curves of experiments in which the specimens failed brittle are simulated by FEM and the stress state at the time of failure is analyzed. The calculated probabilities of cleavage fracture are adapted to the experimental distribution using the maximum likelihood method (ML, [31]-[33]).

3.4. Prediction of fracture mechanical properties

Tests with fracture mechanics specimens are simulated to determine fracture toughness values. Here, the material behavior is described by the parameters of the implemented damage models that were previously identified from the SPT. The evaluation of the stress state in the fracture mechanics specimen provides the relation between Weibull stress and fracture toughness values in the brittle and the transition region, which allows the comparison with the Master Curve [34]. The determination of fracture mechanical parameters by numerical simulations of conventional fracture mechanics tests is based on the hypothesis that the crack initiation both in SPT specimens as well as in fracture mechanics specimens is accurately described by the same material models. In the brittle and transition region, critical fracture toughness values K_{Ic} are calculated from J-integral values if the Weibull stress reaches 5%, 50% and 95% probability of cleavage fracture.

4. Application and results

4.1. Identified Hardening Parameters

The explained identification strategy was applied to determine yield curve parameters from load-displacement curves of SPTs carried out for the two materials, both in non-irradiated and irradiated state, at different temperatures.

The influences of test temperature and irradiation level on the hardening characteristics of the reactor steels are clearly visible in the measured load-displacement curves of SPT [4][5]. They are also found in the identified yield curves. Lower temperatures and higher irradiation levels lead to a significant increase in yield stresses in the entire strain range. Figure 1 shows the identified initial flow stresses for the material JFL. The results for the material JRQ are not shown here as they are comparable in quality; however JRQ shows a much higher sensitivity to radiation than the steel JFL. The identified values agree well with data measured with standard tensile test.

4.2. Determined Weibull Parameters

Weibull parameters were determined for those temperatures and irradiation levels, respectively, for which the tested specimens failed in a brittle manner. Using the maximum likelihood method, unreasonable high Weibull modules were obtained for some test series. Therefore, it was decided to set the Weibull module to a constant value of m=30. The parameters of the original Beremin model were identified for reference purpose. Figure 2 represents the determined Weibull reference stresses for the material JFL.

Both the parameters of the original and the modified Beremin model show dependencies on irradiation level and test temperature. The influence of temperature on the Weibull reference stress is best visible for the non-irradiated materials: Within the same irradiation level, the specific Weibull reference stresses decrease for higher test temperatures.

4.3. Critical Fracture Toughness values

Subsequent to the identification of the yield curves and the damage parameters critical fracture toughness values were indirectly quantified by numerical simulation of fracture mechanics tests. The developed non-local ductile damage model was used in combination with the original Beremin model or the modified version after Bernauer to calculate the probability of cleavage fracture.

The fracture toughness values from FEM calculations of CT specimens using the identified parameters are shown in Figure 3 for the non-irradiated material JFL. In the brittle region and the ductile region, the calculated values agree well with experimental results. For the transition region, the calculated fracture toughness values and their scatter are clearly too small.

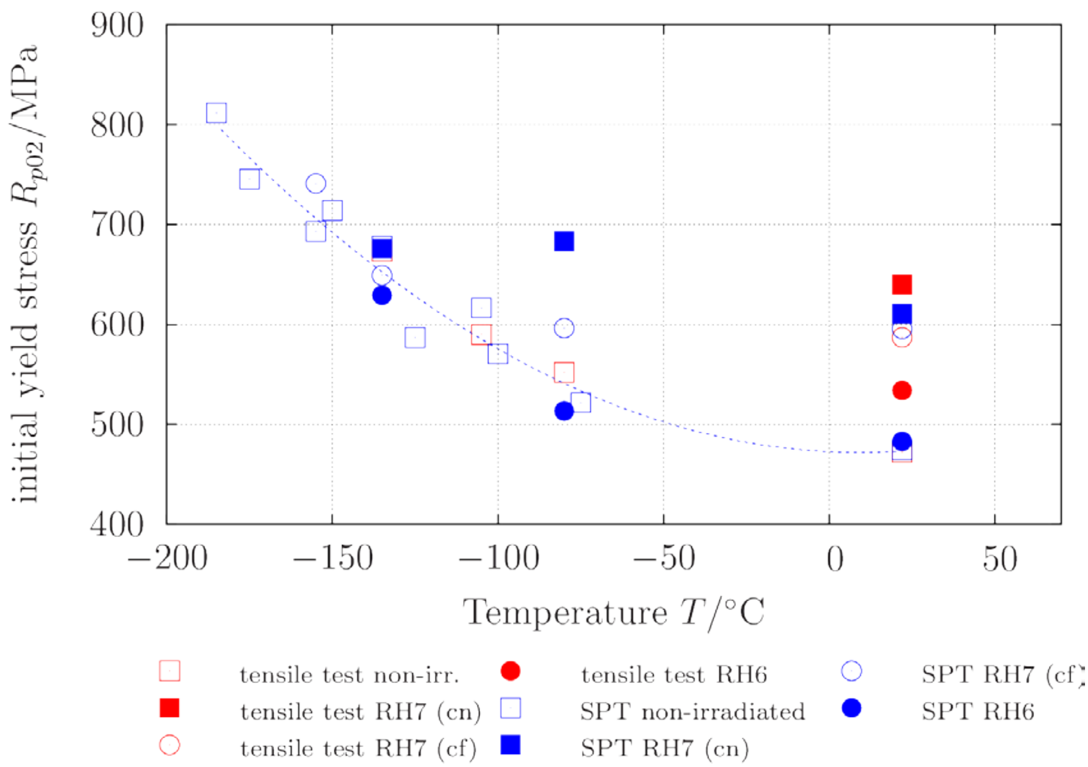

Figure 1: Initial yield stresses identified from the SPT (material JFL; irradiation levels: non-irradiated, RH6, RH7cf/cn)

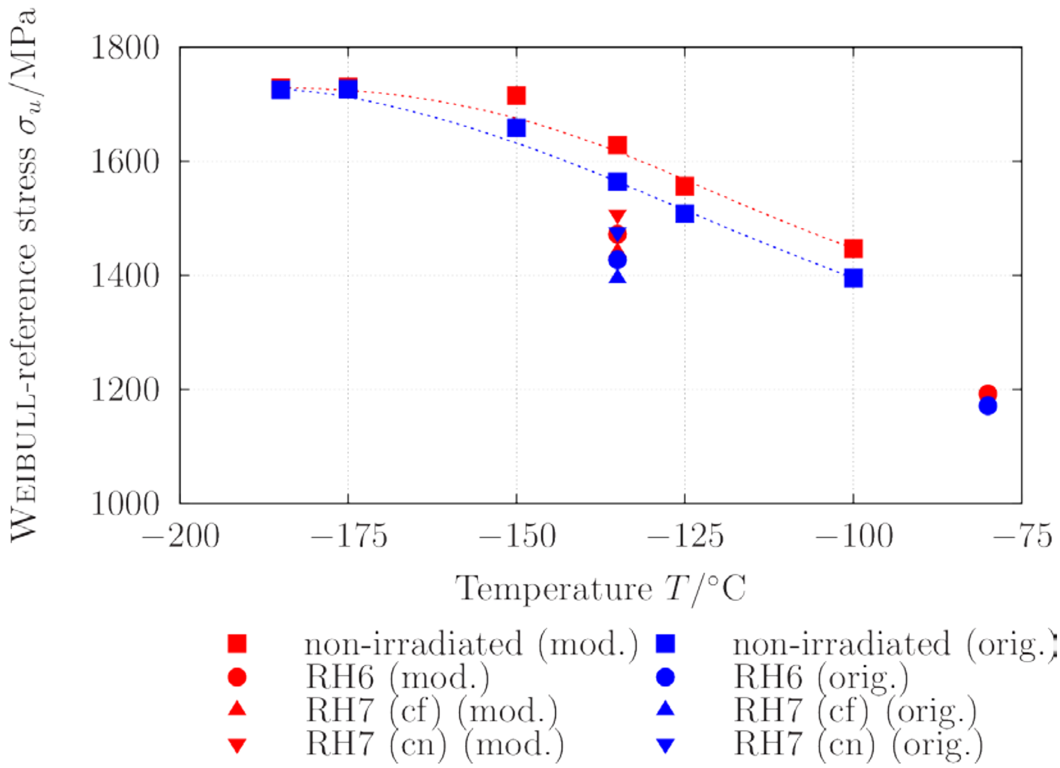

Figure 2: Weibull reference stresses identified from the SPT (material JFL; irradiation levels: non-irradiated, RH6, RH7cf/cn)

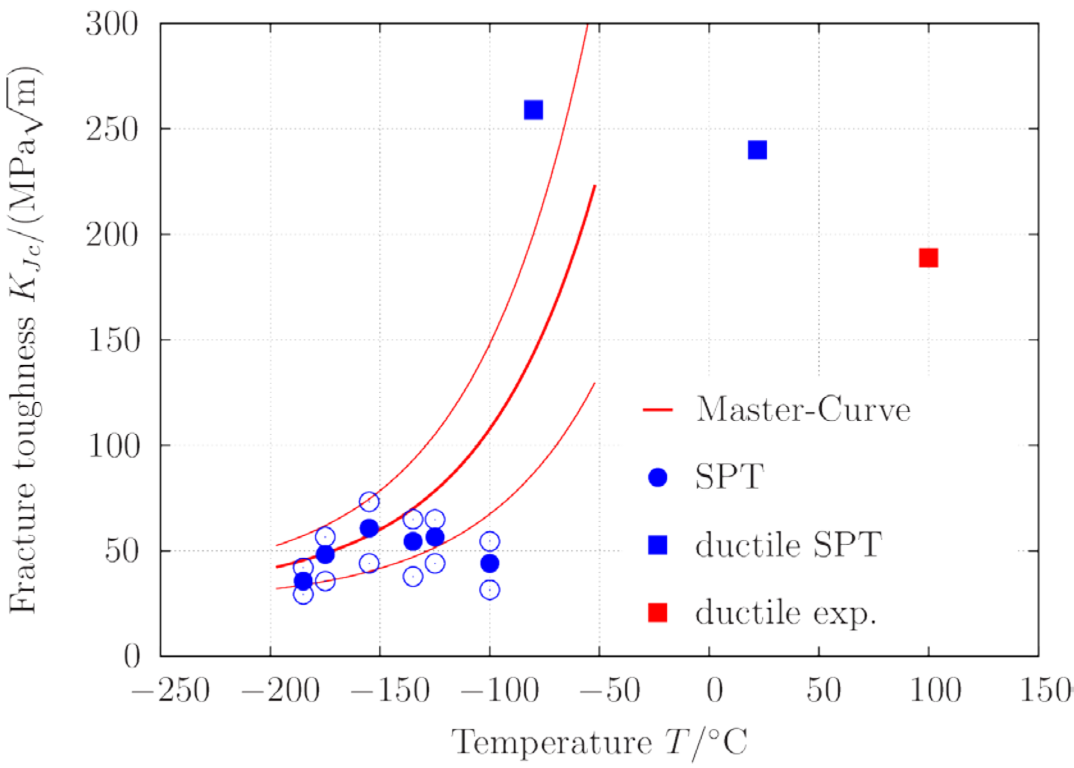

Figure 3: Fracture toughness values for the non-irradiated material JFL

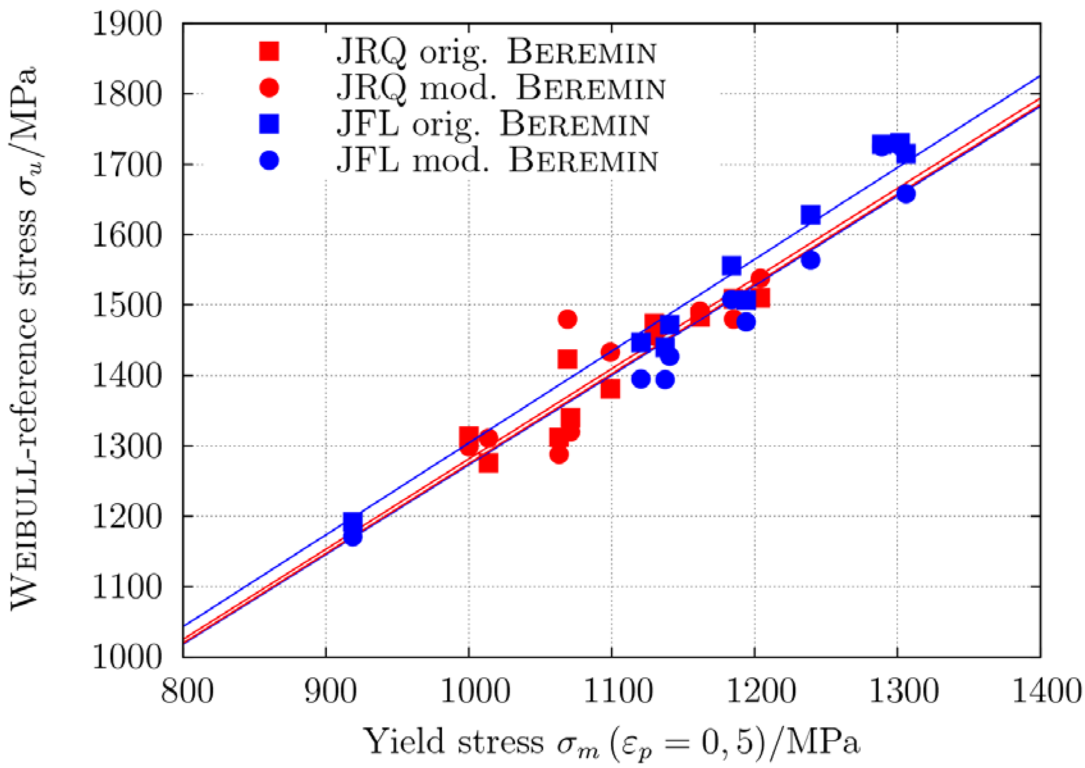

Figure 4: Relation between identified yield stresses and Weibull reference stresses

5. Discussion and conclusions

The parameters of both Beremin models clearly show dependencies on irradiation level and test temperature. In the relevant range of the load-displacement curve of the SPT, large parts of the specimen are subjected to a biaxial stress state which is characterized by approximately equal first and second principal stresses. Accordingly, the maximum principal stresses at the onset of void coalescence and consequently the determined Weibull reference stresses are mainly determined by the current yield stress of the material. Figure 4 shows the almost linear relationship between calculated Weibull reference stresses and identified yield stresses. The strong influence of the test temperature and irradiation level on the hardening properties of the matrix material thus transfers to the particular Weibull reference stresses: for higher temperatures, the Weibull reference stresses decrease. This result is consistent with the temperature dependence of principal stresses leading to cleavage fracture that were experimentally determined on notched tensile specimens [35]. Note that there are several temperature-dependent modifications of the Beremin model, e.g. [36]-[38]. However, in these modifications the Weibull reference stress must be increased with higher temperatures to get reasonable results, which lacks a micromechanical motivation [39] and contradicts with our results.

The predicted fracture toughness values agree well with experimental results in the brittle region and in the ductile region. In the brittle-ductile transition region, the values determined from the SPT cannot be transferred to the fracture mechanics specimen. The calculated fracture toughness values are much smaller than the experimentally determined values. It is therefore questionable whether the assumptions made in the Beremin model are sufficient to capture size effect and influence of stress triaxiality. Particular in the transition region, the assumption of the failure of the whole structure by the unstable crack growth of a micro-crack (weakest link assumption) seems to be not justified for the fracture mechanics specimen.

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