ON THE EVALUATION OF INTERFACIAL CRACK INITIATION BY MEANS OF FINITE FRACTURE MECHANICS

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ABSTRACT

The evaluation of the degree of criticality of crack nucleation, initiation and propagation in the vicinity of bimaterial notches and the reliability of the junctions is a demanding problem, since bimaterial wedge or notch configurations are identified as potential weak locations. The singular character of the stress field at cracks or notches can be investigated analytically or numerically, the angle of the direction of potential crack initiation may also be determined, but the decisive question is whether crack initiation and subsequent crack arrest will really occur or not. An essential requirement in this context is a dependable criterion for crack nucleation. For that aim, the hypothesis of Leguillon is modified. Herein, the crack is assumed to be initiated and to grow if and only if both the released energy and the local stress reach critical values. Thus, simulating virtual crack growth along an interface, the integrity of the joint is revisable and finite characteristic crack lengths can be determined and assessed.

This concept is transferred to a bimaterial interface configuration of a thin layer on a substrate under high thermal loading, as required for modern high temperature Solid Oxide Fuel Cell Stacks. Within the fuel cell stack, multilayered ceramic components have to be embedded in metallic interconnect frames. Due to the mismatch of the individual layers and the interconnect in the mechanical and thermal properties, the joints, as regions of material and geometrical discontinuities, are highly demanded and are potential weak locations.

1 SIMULATION PROCEDURE

As an approach to the assessment of bimaterial joints, the simulation of hypothetical cracks is required. Considering virtual crack growth along the interfaces, strain energy release rates can be calculated numerically. By convention, the symbol $\mathcal{G}$ designates the energy release rate. On the other hand, $\mathcal{G}_{\text{crit.}}$ denotes the critical energy release rate or fracture toughness as the material's resistance to crack growth. The calculation of energy release rates can be carried out by serveral methods.

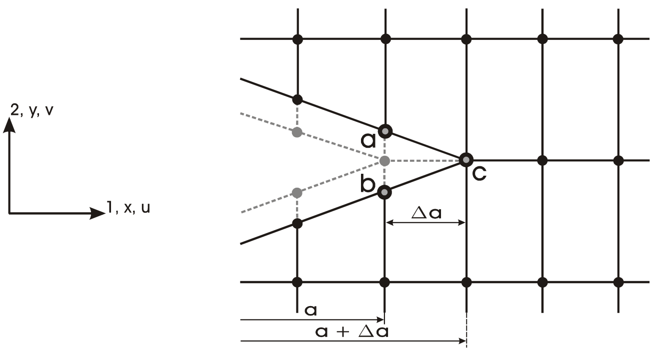

Figure 1: Calculation of energy release rates using the method of Rybicki and Kanninen.

The energy release rate can be calculated by the crack closure integral according to Irwin [1], or in an approximate manner by the method of Rybicki and Kanninen [2], see eqn. (1). Herein the integrals are determined with the help of the nodal forces and displacements which are obtained directly from the finite element analysis where the crack propagation process is simulated using the node release technique. Then, the energy release rate is given by:

$\mathcal{G} = \mathcal{G}_I + \mathcal{G}_{II}$ with:

Irwin 1957:

$$\mathcal{G}_I = \lim_{\Delta a \to 0} \left[\frac{1}{2\,\Delta a} \right] \int_0^{\Delta a} \sigma_y \, u_y \, dx \quad \text{and} \quad \mathcal{G}_{II} = \lim_{\Delta a \to 0} \left[\frac{1}{2\,\Delta a} \right] \int_0^{\Delta a} \tau_{xy} \, u_x \, dx$$

Rybicki/Kanninen 1977:

$$\mathcal{G}_I = \frac{1}{2\,\Delta a} F_{y_c} \left(v_a - v_b \right) \quad \text{and} \quad \mathcal{G}_{II} = \frac{1}{2\,\Delta a} F_{x_c} \left(u_a - u_b \right) \tag{1}$$

In these relations, the indices I and II indicate the crack opening modes. For a crack extension of Δa as shown in figure 1, $\mathcal{G}_I$ for the opening mode I is calculated from the vertical nodal forces of the node C and the relative displacements of the nodes A and B in vertical direction caused by the virtual crack propagation. In analogy, the energy release rate $\mathcal{G}_{II}$ for the sliding mode II is determined by the nodal forces and the relative displacement in the horizontal direction. In sum, these two components represent the total energy release rate $\mathcal{G}$. Simulating the crack growth, the nodes C have to be untied step by step. Thus, the crack is extended virtually in each single step by an additional length Δa.

Two common criteria for the assessment of interface crack onset at notches exist side by side: A stress-based and an energy-based criterion. The stress-based criterion predicts fracture, if the maximum value of the interface tensile stress exceeds the interface strength:

$$\sigma_y \geq \sigma_{y,\text{crit.}} \, . \tag{2}$$

Due to the singular stress field in the bimaterial notch situation considered here, in any case, the material or the interface strength is exceeded in some regions which should lead to fracture according to the strength criterion, even if the load is very small. Although a notch is a privileged location for crack initiation obviously not every small load applied at a notch causes fracture! On the other hand, the energy-based criterion predicts fracture if the energy release rate $\mathcal{G}$ exceeds its critical value, the toughness $\mathcal{G}_{\text{crit.}}$:

$$\mathcal{G} \geq \mathcal{G}_{\text{crit.}} \, . \tag{3}$$

In terms of eq. (3), the toughness of the interface and of the joined materials is taken into account. Assuming a given situation with a notch without any initial crack, the energy release rate is zero. Thus, according to the energy criterion in the given infinitesimal form, no crack nucleation would ever be predicted. Nevertheless, notches are critical locations for crack formation.

In order to derive a more satisfying predictive concept for fracture, the concept of finite fracture mechanics introduced by Hashin [3] is adopted. Herein, the hypothetical instantaneous onset of cracks of finite length is considered. It is checked whether such cracks are possible from both points of view, exceeded strength and sufficient energy released. In accordance with the hypothesis of Leguillon [4], the two criteria taken together form a sufficient condition of fracture. Satisfying both, strength and toughness criterion simultaneously, a characteristic length of crack onset can be determined. In this case the total released energy E for the hypothetical crack of length a has to exceed the integrated fracture toughness,

$$E \geq E_{\text{crit.}} \quad \text{with} \quad E = \int_a \mathcal{G} \, da \quad \text{and} \quad E_{\text{crit.}} = a \, \mathcal{G}_{\text{crit.}} \, . \tag{4}$$

2 ANALYSIS MODEL AND APPLICATION

As an example of application, a Solid Oxide Fuel Cell (SOFC) stack is considered in this investigation. It is characterized by a planar, anode supported design. The membrane electrodes assembly (mea, representing the functional layers: anode, electrolyte and cathode) is a sintered composite consisting of three layers of ceramic materials. Because of the anode supported design, the anode layer is a relatively thick porous cermet, the electrolyte is a thin film with a thickness of about 1/150 of the anode thickness. The cathode is a thin porous ceramic layer. Even a slight mismatch of the individual sintered layers of the mea in their coefficients of thermal expansion leads to highly demanded joining areas since the applied temperature loads are considerable ($\Delta T = 800° C$). In addition, the different shrinkage behaviour of the materials during the manufacturing sequence causes further problems, for detailed information see Müller et al. [5]. Nevertheless, it is essential to maintain the mechanical integrity because the joints adopt the function of gas tightness.

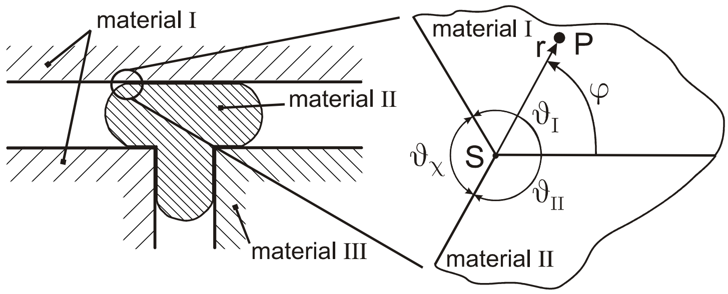

Figure 2: Sealing joints of the application investigated as bimaterial joint.

Focussing the investigations on the sealings, these junctions are scrutinized as they are seen to belong to the most critical regions of the whole SOFC-stack. As fig. 2 illustrates, the local stress concentration regions can be idealized as bimaterial notches. The structural mechanical assessment of these bimaterial notch situations is the objective of the work presented. The analyses are based on the assumption of isotropic, linear-elastic behaviour of the involved materials. The local stress fields which have to be analyzed in a first step, see Müller et al. [6], show an singular asymptotic behaviour. The singular stress field at the investigated bimaterial notch differs from the well-known crack tip singularity in the exponent and is mainly affected by the geometry and the combined materials. Simulating the initiation of hypothetical cracks and their virtual growth along the bimaterial interfaces, the criticality of potential cracks can be estimated.

In order to assess a virtual potential crack along the interfaces between the glass ceramic sealing and the interconnect respectively the electrolyte layer, a characteristic lay-up of a SOFC-stack is chosen for the simulation by finite element analysis as shown in fig. 3.

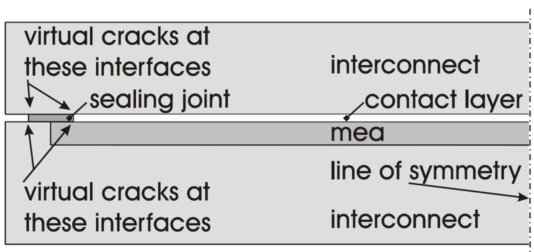

Figure 3: Slice (not in scale) of the considered application and the virtual crack positions.

As a composite structure of thin ceramic layers, the membane electrodes assembly (mea) is embedded in a frame within the interconnect. The simulations presented are performed for a thermal load by which the representative structure of fuel cell stack is cooled down from the service temperature (800° C) to room temperature. The investigations are concentrated on crack growth along the interface, since in general the interface toughness is lower than the fracture toughness of the joined materials, see experimental studies by Malzbender et al. [7]. The corresponding FE-mesh contains approximately 130.000 degrees of freedom. Along the lower edge of the interconnect, no vertical displacements are allowed, and along a vertical line at the middle of the sealing joint the horizontal displacements can be suppressed for symmetry reasons.

3 ASSESSMENT OF JOINTS

Applying Leguillon's hypothesis to the SOFC-stack, first of all a specific geometrical configuration is investigated as a reference. Therefore, a joint with joining angles $\vartheta_\chi = 90°$ with a layer thickness of the joining material of 0.25 mm and a width of 10 mm is assumed. In this case, virtual crack growth along the interface between the glass ceramic sealing joint and the interconnector plate consisting of steel, is simulated. Fig. 4 contains the resultant curves, the amount of the released energy and the resultant stresses compared to the critical curves of each case. The underlying problem is a virtual crack on the top left position corresponding to the considered glass/interconnect interface, see fig. 3.

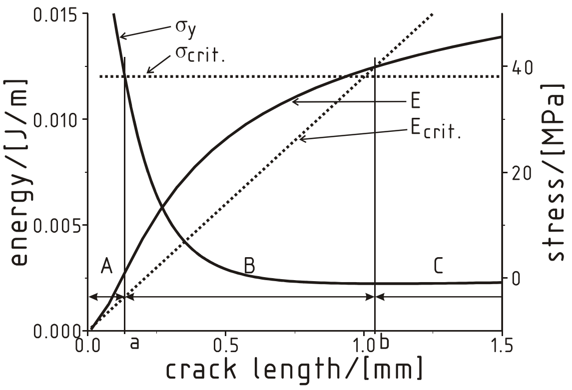

Figure 4: Assessment of joints: reference configuration, 0.25 mm joint thickness.

Three ranges of crack lengths can be distinguished: A range A, where first only the strength criterion, then both criteria are satisfied simultaneously. Here the nucleation of a crack is predicted in accordance to finite fracture mechanics. Up to a crack length a, the admissible stress is exceeded while the amount of the energy released surpasses the critical value. Consequently, a crack with this length a is initiated due to the singular stress field at the underlying 90°-bimaterial notch and due to the fact that sufficient energy is available. During the subsequent range B the energy necessary for fracture is available furtheron. Considering the stress situation with a crack onset, the singular stress field moves with the propagating crack tip. As a consequence, both criteria are again satisfied, thus representing a range of instable crack growth. Crack arrest is expected in range C at a length b, because the energy required for crack propagation is no longer available, though the strength is still exceeded locally. So, in short, in the case of the reference interface, crack arrest at a characteristic length of about b = 1 mm is expected.

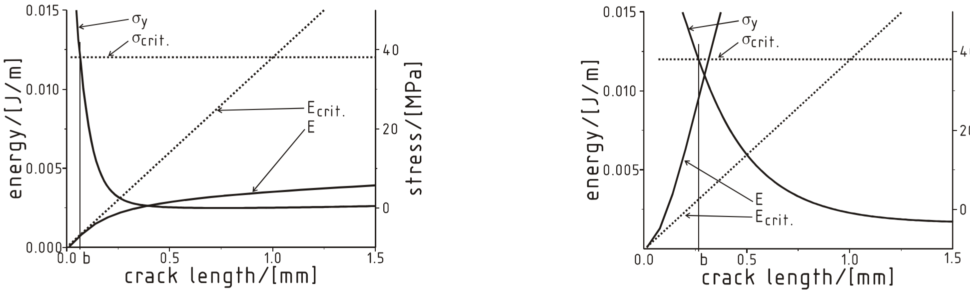

Figure 5: Assessment of joints, joint thickness 0.125 mm (left) and 0.5 mm (right).

Further investigations are concerned with the effect of the joint thickness. Results are presented in fig. 5. The virtual crack is assumed to grow along the top left interface (interconnect/glass), the joint thickness of the reference geometry, fig. 4, is 0.25 mm. Reducing the joint thickness to its half (0.125 mm; fig. 5, left), the joint is predicted to be significantly more resistant to crack nucleation. While for the reference configuration cracks with a characteric length are expected, no crack initiation is expected here, as the energy criterion is never satisfied. Therefore, the energy necessary for the creation of new crack surfaces is not available for any virtual crack length. Thus, for the case of a thin joint, no crack occurrence is expected, while a characteristic crack stopping at approximately 1 mm is predicted for the reference configuration with a joint thickness of 0.25 mm.

Thicker joints do not improve the junction, as the graphs on the right hand side of fig. 5 demonstrate. Herein, a joint is simulated with a thickness of 0.5 mm, twice the reference thickness. This joining situation is the most critical configuration investigated within this work. From the beginning of the virtual crack growth, both criteria are satisfied simultaneously. The strength criterion is fulfilled because of the singular stress field in the vicinity of the underlying 90° bimaterial notch. Together with the simultaneously exceeded critical value of the released energy, the condition sufficient for crack nucleation is met. A crack is born and is expected to grow onward. Since the initiated crack will grow as long as the necessary energy is available, no crack arrest will occur. Over the investigated range up to half the joint width (5 mm) no section point between the curve of the released energy and its critical value curve can be observed. Thus, no crack arrest can be expected in this case.

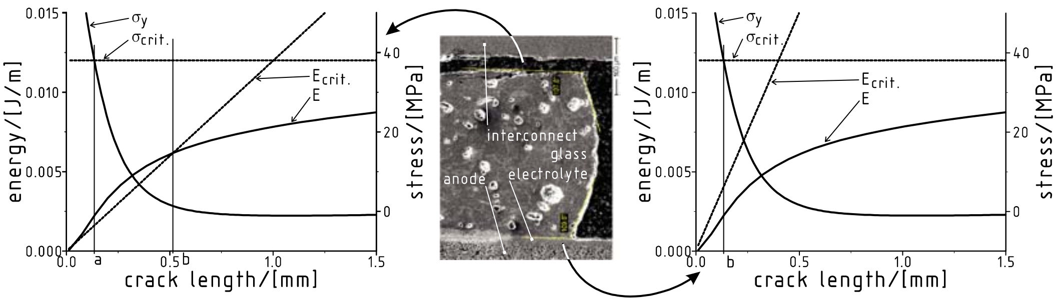

Figure 6: Assessment of joints, interface glass ceramic/metal (left) and glass ceramic/ceramic.

At the right hand side of the sealing (optical micrograph, in the centre of fig. 6), two interfaces can be distuinguished: An interface between glass ceramic sealing and the metallic interconnect at the top right position and an interface between the more similar materials glass ceramic sealing and ceramic electrolyte layer. For a crack at the interface between the glass ceramic sealing and the interconnect (fig. 6, left picture), the graph shows a behaviour similar to the reference interface at the top left position discussed before. In contrast to this, at the bottom right position, the interface between the electrolyte layer and the glass ceramic sealing (fig. 6, right), the strength criterion is exceeded at every virtual crack length up to a virtual crack length b. Within the crack initiation range, this is due to the singular stress field in the vicinity of the bimaterial notch. Subsequently, the cause is the stronger crack tip singularity. However, since the energy criterion is not satisfied simultaneously, the energy release would be insufficient for fracture. Thus, only one criterion necessary for fracture is met. For that reason, no crack initiation is expected so that this interface is regarded as not critical. This theoretical perdiction is confirmed by the sectional micrograph of the entire right side of the sealing joint, depicted in the middle of fig. 6. As two ceramic materials are connected at this interface, the interface toughness ($3\ 10^{-2}$ N/mm) is higher than that of the interfaces between the dissimilar materials metallic interconnect and ceramic glass ($1.2\ 10^{-2}$ N/mm).

4 CONCLUDING REMARKS

A fracture mechanical assessment of the joint integrity has been presented using the hypothesis of Leguillon. It enables us to simulate crack nucleation. The results correspond in excellent way to experimental observations. Thereby, characteristic lengths of the cracks can be determined and an assessment of dependences of the degree of criticality of junctions on the combination of materials and on the joint geometry is possible.

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