Numerical and Experimental Fracture Mechanics Based Optimization of the Crack Resistance of Carbon/Carbon to Copper Interfaces


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Abstract

The optimization of CFC/Cu-interfaces for plasma facing divertor components in thermo-nuclear fusion reactors is proposed and demonstrated via an integrative numerical-experimental approach mainly comprising a macro-scale to micro-scale finite element modeling technique together with fracture mechanics tests. Results obtained by finite element analyses of real-scale CFC flat tile divertor components under high heat flux loading conditions are verified by the findings of tests in an ion beam high heat flux facility. From those macro-scale FE models of the full component the loading conditions are derived for micro-scale FE models that incorporate principal details of the micro-structured CFC/Cu-interface such as topological features of the laser structured CFC surface, the local compositional gradient at the interface due to phase formation during the joining process as well as advanced material descriptions for those phases. Locally acting dissipative mechanisms such as ductile damage and cleavage are explicitly accounted for in the FE models which in turn at the macro-scale in 3-point bending fracture mechanics experiments increase the fracture toughness of the CFC/Cu-interface. This way the functional dependence between the micro-scale topology and material parameters of the CFC/Cu and the macro-scale fracture toughness is extracted and an optimized parameter set is proposed. Laser structuring and joining via Active Metal Casting are accordingly adapted and fracture mechanics experiments on CFC/Cu-specimens clearly demonstrate the applicability of the proposed optimization strategy.

Keywords

Nuclear fusion, divertor, CFC/Cu interface, optimization

Introduction

Wendelstein 7-X is an experimental nuclear fusion reactor currently being built in Greifswald, Germany [1]. Its purpose is to evaluate the main components of a future fusion reactor. Wendelstein 7-X itself is not yet an economical fusion power plant.
The goal of fusion reactors is to produce energy like in the sun. To ignite the plasma for the fusion process it has to be heated to 100,000,000 Kelvin and is enclosed in magnetic fields preventing the plasma from colliding with the reactor walls. Figure 1 shows the basic design of the reactor.

In order to extract energy from the plasma ions are directed against divertor units converting the energy of the particles to heat. The water cooled divertor units are subjected to very high heat fluxes, high temperatures and radiation. The divertors are designed in layers of different materials. Only a small number of materials can sustain being on the hot side with up to 2300 K. One of them is carbon fiber reinforced carbon (CFC).

Figure 2 depicts the basic design of a CFC-divertor plate with the metal components made of copper and copper alloys including the cavity for the cooling water. The critical zone within the component is the interface layer connecting the copper basis with a ceramic layer (CFC). Both materials have different mechanical properties, first to mention the thermal expansion coefficients. Since the divertors are mainly exposed to thermal loads, which occur also during the manufacturing processes, the interface stresses results from different thermal strains in the materials. The components of the interfacial traction are tension perpendicular to the interface and shear, comparable to the crack modes I und II in fracture mechanics.
By assuming elastic behavior for both of the materials and a planar interface this gives a singular stress field along the free edges of the interface when the component is subjected to thermal loading. This is well known as the free edge effect.

Practical applications clearly show that a planar interface between the copper and CFC sections is not able to withstand the thermal loads applied to the component. The interface fails beginning on the free edges of the divertor.

Fig. 3: Micro structuring of the interface.

In order to produce a reliable joining of the metal and CFC Plansee developed a micro (μ-) structured interface. Figure 3 on the left side shows the result of the first manufacturing step where a laser beam is used to burn conical holes into the CFC-surface. In a next step the CFC-surface has to be activated since copper and CFC can not directly form a bond. Thin titanium sheets are melted above the μ-structured CFC covering the surface with a compositional gradient layer primarily consisting of titanium carbide (TiC). After this step liquid copper is being casted onto the μ-structured and activated surface (Active Metal Casting / AMC® [2]) forming copper needles reaching into the CFC. The right side picture of figure 3 shows a cross section of a needle interface region (here a curved divertor interface is shown). After the casting process the copper surface is machined and joined with the rest of the divertor structure.

As already mentioned a reliable interface is crucial for operating the reactor. This directly leads to the problem of finding the optimized shape and composition of a μ-structured interface.

**Optimization Strategy**

The objective is to find the toughest possible interface. The free edge effect as well as the porosity within the CFC leads to high local stresses even causing local damage within a limited length scale. The interface must be able to stop a further growth of debonded or damaged areas. This approach leads directly to the energetic formulation known from fracture mechanics and discussed composite interfaces e.g. in [3].

A crack - or in our case a damaged interface - remains stable if the elastic energy release rate is smaller than the energy needed to propagate the crack or damaged region. The elastic energy release rate depends on the geometry, the material characteristics and the loading conditions. In the case of the divertor the interface layer is thin compared to the other dimensions of the component. Therefore, we assume that the μ-structured interface layer has only minor influence on the overall energy release rate. This way the optimization process can be reduced to the problem of finding a type of μ-structure with maximum energy absorption when being torn apart.

The main optimization parameters are: (i) needle diameter at the basis of the needles, (ii) needle length, (iii) distance between needles in a hexagonal pattern (clearance of needles), (iv) thickness of the activation layer (TiC).
The optimization setup was planned using the DOE (Design of Experiment [4]) approach. Approximately thirty different geometrical designs were derived.

The optimization was planned to be performed numerically using the finite element method (FEM). A realistic representation of the interface must incorporate details such as the topological features and the mechanical properties of all components. Since it is not possible to model a complete divertor with its µ-structured interface a hierarchical modeling strategy was chosen. One type of model represents the divertor (macro scale) which is needed to extract realistic interface loads. A second type of models comprises unit cell models representing only a small section of the µ-structured interface layer but doing this in a geometrical detailed manner. The typical length scale of the micro scale models is the diameter of the copper needle.

**Macro Scale Simulation**

Results obtained by finite element analyses of real-scale CFC flat tile divertor components under high heat flux loading conditions were verified by the findings of tests in an ion beam high heat flux facility [5]. From those macro scale FE models of the full component the loading conditions are derived for micro-scale FE models.

A macro scale model is shown in figure 4. The contour plot displays principal strains. The enlarged detail in figure 4 shows the different layers of the divertor near the interface consisting of CFC, OFHC Cu and CuCrZr. The OFHC Cu layer shows a low yield stress. The maximum strain values can be detected in the OFHC Cu layer mainly driven of plastic deformation. The main output from macro scale models is an adequate representation of normal und shear strains within the interface layer near the free edges of the component. These values are used for the correct loading of the models on the micro scale level.

![Fig. 4: Predicted strain results of a macro model under high heat flux.](image)

**Micro Scale Simulation**

In order to maximize the energy absorption of the interface all important irreversible mechanisms of the constituent materials must be described in the finite element model. These are (i) plastic yielding of the metal phase (OFHC Cu), (ii) brittle behavior (cleavage) of the TiC layer, and (iii) inelastic orthotropic material behavior of the CFC.
The simulations on the micro scale level are performed using a unit cell approach. Figure 5 shows the geometry of the unit cell model as well as the material sections. On the right hand side the loading of the cells is indicated with a red arrow for tensile loading perpendicular to the interface plane and a green arrow for the shear loading.

Assuming a hexagonal arrangement of the needles within the interface plane it is sufficient to model only a quarter of two needles, see figure 5. By adopting periodic boundary conditions the unit cell model describes a uniformly loaded μ-structured interface.

Figure 6 shows all possible deformation patterns of a unit cell model:

a) tension/compression perpendicular to the interface plane (direction 2)

b) shear in the 1-2-plane

c) tension/compression direction 3

d) tension/compression in direction 1
The simulations were performed using the commercial FEM package ABAQUS [6]. This code offers different material models for inelastic material behavior. The metal is described using a standard von Mises plasticity formulation in combination with isotropic hardening. The TiC layer is described using a constitutive formulation for brittle materials including damage.

The behavior of the CFC cannot be described with standard material laws as available in ABAQUS. Therefore, a specific material model was developed and implemented describing the nonlinear orthotropic behavior using a continuum damage formulation based on a homogenized material description [7]. Figure 7 and 8 illustrate the strongly orthotropic features of the material. The example shows data for the CFC-type NB31. The main orientation of the fibers is perpendicular to the interface plane (direction 2) which is also the direction of the largest heat flux. The material strength under loading in direction 2 is almost one magnitude higher than the value for direction 3. In order to capture instable material behavior (softening) a dynamic finite element formulation was selected.

![Fig. 7: CFC behavior, direct stresses.](image1)

![Fig. 8: CFC behavior, shear stresses.](image2)
Results of the Micro Scale model

Figure 9 shows the predicted interface characteristics in terms of homogenized stress over strain perpendicular to the interface plane. The curves show a kink at a strain level of 0.05%. This corresponds to the onset of yielding in the OFHC Cu layer. Furthermore, all curves - representing different $\mu$-structured interfaces - climb to failure stress levels between 100 MPa and 120 MPa before dropping down to low values.

![Figure 9: Predicted interface characteristics in terms of normal stress over strain.](image)

The objective of the optimization problem was defined regarding an maximization of the energy absorption. Figure 10 shows corresponding results. On the left side diagram the energy absorption per unit cross section is shown. Again, the curves represent different interface designs as shown on the right side of figure 10. Red zones indicate material failure of the CFC. In the diagram all curves follow the same path up to energy levels of 0.16 mJ. Up to this value energy absorption is dominated by plastic deformation of the OFHC Cu basis, which is nearly the same for all investigated designs. Energy gains above the value of 0.16 mJ characterize the absorption capability in the interface.

![Figure 10: Predicted energy absorption of different interface designs.](image)
From the three pictures on the right side of figure 10 it can be seen that long slim needles a) are better than short ones b). Even worse for the absorption is a large clearance between the needles c).

Figure 11 illustrates the energy absorption of the different phases of an interface design variant. The red curve a) in the diagram describes the total energy absorption. The orange curve b) shows the contribution of the OFHC Cu which is dominant up to a strain of 0.25%. The green curve c) stands for the CFC and the last curve d) for TiC. The sudden jump at an almost constant macroscopic strain level resembles the sudden failure of the interface (indicated by the arrow in fig.11).

The Young’s Modulus of the CFC in direction of the needle axis is larger than the Young’s modulus of the needle itself. In case of an intact interface the needles transfer only a little percentage of the total load. With a proper interface design failure occurs near the basis of the needles. The failure strength is reached and the load carrying capacity drops immediately. Since the needles are ductile a connection between metal and CFC remains in the conical region and further energy absorption is possible and can even stop the growth of the interface failure or damage zone.

![Fig. 11: Predicted energy absorption of different constituents.](image)

The contour plot of the unit cell on the left side of figure 11 shows the CFC damage indicator SDV3 (i.e. stiffness degradation) for the tensile loading in the direction of the needle. On the right side the state variable SDV7 represents damage due to interface shear loads.

The optimization process finally defined a new ideal geometry for the µ-structured interface defining length, base diameter, needle spacing, and thickness of the TiC layer.

Besides varying geometrical features of the needles also variations in the mechanical properties of the interfacial phases were investigated. In particular the ratio between the strength of the CFC and the yield stress of the Cu needles plays an important role. Increasing the yield stress in the needles can lead to lower energy absorption when the needles are torn out of the CFC without being plastically deformed.
Verification by 3-Point Bending Tests

On the basis of the results of the numerical optimization different prototype µ-structured interfaces were tested [8]. In 3-point bending fracture mechanics experiments the differences in fracture toughness between different interface types could be proven. The experiments show that long slender needles combined with small spacing are favorable for energy absorption. Furthermore, the experiments show a strong dependence on variations in the copper yield stress or the CFC tensile strength.

In figure 12 a experimental setup for a 3-point bending test of a CFC/Cu specimen is shown.

Fig. 12: Setup of a 3-point bending test.

This way the functional dependence between the micro scale topology and material parameters of the CFC/Cu and the macro-scale fracture toughness can be extracted.

The results of the fracture mechanics experiments on CFC/Cu-specimens demonstrate the applicability of the proposed optimization strategy resulting in an optimized parameter set for an advanced divertor designs. Different steps in the manufacturing process, such as laser structuring and joining via Active Metal Casting, were accordingly adapted.

Conclusions

In this contribution the authors present an optimization strategy for a µ-structured interface of a divertor used in a nuclear fusion reactor. The interface connects a CFC with a metal component made of Cu. The assembly is subjected to high heat fluxes and large thermal strains occur due to a mismatch in the thermal expansion coefficients of CFC and Cu.

The objective of the optimization is defined as to maximize the quantity of energy absorption during failure of the interface. A tough interface absorbs a high amount of energy und thus helps to stop the growth of damaging zones or propagating cracks.

In current interface designs of CFC/Cu divertor components different length scales can be identified and are identified to have a direct effect on the modeling strategy using finite element analysis. Macro scale simulations characterizing the entire component deliver strain fields in the interfacial region. These strain fields serve as loads of the models on the micro scale level the latter describing the µ-structured interface in a detailed manner. A unit cell approach is used for analyzing the energy absorption of the micro structured interface.
A set of optimized interface parameters is used in real-scale prototypes and corresponding 3-point bending tests are performed. The results of the tests demonstrate the applicability of the proposed optimization strategy.

References