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# Modelling of thermal shock experiments of carbon based materials in JUDITH

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## Abstract

The interaction of hot plasma with material in fusion devices can result in material erosion and irreversible damage. Carbon based materials are proposed for ITER divertor armour. To simulate carbon erosion under high heat fluxes, electron beam heating in the JUDITH facility has been used. In this paper, carbon erosion under energetic electron impact is modeled by the 3D thermomechanics code 'PEGASUS-3D'. The code is based on a crack generation induced by thermal stress. The particle emission observed in thermal shock experiments is a result of breaking bonds between grains caused by thermal stress. The comparison of calculations with experimental data from JUDITH shows good agreement for various incident power densities and pulse durations. A realistic mean failure stress has been found. Pre-heating of test specimens results in earlier onset of brittle destruction and enhanced particle loss in agreement with experiments. © 2004 Elsevier B.V. All rights reserved.

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#### 1. Introduction

Due to plasma instabilities in tokamaks, off-normal events such as plasma disruptions, ELMs or VDEs (vertical displacement events) may take place. During these events, the extremely high heat fluxes impinging on plasma-facing materials may cause strong erosion and damage of the materials. Both erosion and material damage result in a reduction of the lifetime of plasma-facing components. Additionally, the eroded material contaminates the hot core of plasma. The most intensive heat load is expected in the divertor part of a fusion reactor. Carbon based materials such as fine grain graphite and carbon fiber composites (CFC) NB31 and NS31 are proposed for the divertor armour in ITER next step device.

In order to evaluate the degradation of carbon based materials (CBMs) under high heat loads, the thermal shock experiments using the scanning electron beam facility JUDITH [1–3] have been done. The electron beam was scanned in a triangular mode on the specimen's surface with frequencies f(x, y) = (46.5, 43.4) kHz to get a homogeneously loaded area. The pulse length was varied from 0.5 to 90ms, and the incident current from 50 to 350mA at an acceleration voltage of 120 keV resulting in an absorbed power density in the range of 0.14–7.7 GW m<sup>-2</sup>. The loaded area was  $2 \times 2$  mm<sup>2</sup> for 1–3.5 ms and  $3 \times 3$  mm<sup>2</sup> or  $4 \times 4$  mm<sup>2</sup> for 4.5 ms, respectively. The test materials are fine grain

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graphite (R6650) by Ringsdorfwerke, Bonn, and threedirectional (3D) CFC (NB31) by SNECMA Propulsion Solide, Bordeaux. Before the tests, the samples were cleaned of adherent dust particles in an ultrasonic baths of ethanol for ten minutes and then baked at 170 °C for 4 h to remove volatile species.

Recently obtained experimental results on CBMs show the following [3–5]:

- For graphite: (i) pre-heating reduces the time till brittle destruction (BD) onset, (ii) erosion is higher for pre-heated graphite, (iii) increase of heat load enhances particle erosion.
- For CFC: (i) pre-heating slightly influences the onset of BD and (ii) erosion is higher for pre-heated sample.

In this paper, the brittle destruction of CBMs is modeled using the 'PEGASUS-3D' code [6,7]. The comparison of experimental data with calculations allows us to explain the mechanism of erosion under various incident power densities and pulse durations. The influence of sample pre-heating on the erosion rate and material degradation during thermal shock experiments is studied.

#### 2. PEGASUS-3D code

The erosion of CBMs results from sublimation and solid particle emission. Particle emission caused by thermal stress and crack formation is referred to as brittle destruction, BD [8]. To understand the mechanism of brittle destruction under hot electron impact, the 'PEG-ASUS-3D' code, adapted for JUDITH experimental conditions, is used. The code includes the real graphite structure which consists of grains of different size and different grain anisotropy directions. The code calculates heat transport, thermal expansion, mechanical stress and crack development. The original code has been modified by the introduction of volumetric heating by energetic electrons. Typically the energy deposition of 120 keV electron beam has a maximum placed at a depth of about 60 µm and a total penetration depth of about 120 µm [9].

In the model the graphite sample is a slab cut from the cube of  $200 \times 200 \times 200$  cubic cells, each of  $3-7 \mu m$ size. The grain volume distribution is Gaussian with mean grain volume of 8–10 cells. This corresponds to a mean grain size of  $\sim 7-17 \mu m$ . Due to the anisotropy of thermal expansion and thermal conductivity of individual graphite grains, the cells anisotropically change their sizes during a heating, thus developing the thermal stress in the bonds.

At each time step the thermal stress is calculated and then the generation of new cracks is assumed at those Table 1

Thermomechanical parameters of adjacent cells (ij) at room temperature.

	Perpendicular to the anisotropy axis	Parallel to the anisotropy axis
Thermal conductivity, $\lambda$ (W/mK)	120	24
Young's modulus, <i>E</i> (GPa)	20	4
Coefficient of thermal expansion, $\alpha$ (K <sup>-1</sup> )	$10^{-6}$	$10^{-5}$
Failure stress $\sigma$ ,	0.003-0.005	0.003-0.005

boundaries between grains, where the thermal stress gets larger than the *local* failure stress value. The *mean* failure stress for the grain surface bonds is denoted as  $\sigma_{0s}$ and for internal bonds as  $\sigma_{0i}$ . The  $\sigma_{0i}$  and  $\sigma_{0s}$  are dimensionless values normalized on Young's modulus  $E_1$ .

The Young's moduli  $E_1$  and  $E_2$ , the thermal conductivities  $\lambda_1$  and  $\lambda_2$  and the thermal expansion coefficients  $\alpha_1$  and  $\alpha_2$  are the principal values parallel and perpendicular to the anisotropy axis which denotes the direction perpendicular to the atomic carbon layers (Table 1). Breaking of real graphite preferentially occurs along the surface of the grains. To simulate this process it is assumed that the mean failure stress of internal bonds  $\sigma_{0i}$ is 10 times higher than that for the grain surface bonds  $\sigma_{0s}$ . This value is high enough that the five fold increase of bonds between cells inside the grain, i.e.  $\sigma_{0i} = 50\sigma_{0s}$ , does not influence average erosion and crack propagation. The five times reduction of failure stress of internal bonds, i.e.  $\sigma_{0i} = 2\sigma_{0s}$ , enhances erosion by approximately two times. If the particles are weakly bonded in a grain then it is as easy to break the bonds between particles in that grain as to break the bonds between various grains. In this case, the size of the grains does not significantly influence the eroded particle size. This was confirmed in the calculations.

### 3. Results

Figs. 1 and 2 show the comparison of experimental and calculated surface morphology and cross-section of a graphite sample. For samples both at room temperature and pre-heated to 500 °C, the 3D-PEGASUS calculations show a good agreement with experiments. Even the qualitative agreement of the erosion crater depth with experiments has been obtained (Fig. 3). Although the sample dimension in calculations was remarkably smaller than in experiments, the calculated and experimental crater depths are comparable. The erosion depth is defined as the total volume of dust particles divided by the heated surface area. Heat loads of  $2.4 \text{ GWm}^{-2}$  and  $1.3 \text{ GWm}^{-2}$  on pre-heated graphite





Fig. 1. SEM image (a) and calculated cross-section (b) of graphite R6650. Absorbed power  $P_{\rm abs} = 3.3 \,\rm GW \,m^{-2}$ , pulse duration  $\Delta t = 2 \,\rm ms$ , room temperature, *RT*.

for durations of 4.4 ms result in average erosion depths of 14µm and 6µm, respectively. Taking into account the scattering of the experimental and calculated data, the calculated erosion of 11  $\mu$ m and 7  $\mu$ m for 2.4 GW m<sup>-2</sup> and 1.3 GW m<sup>-2</sup>, respectively, is a rather good correlation with experiments. Despite the approximate values of thermal mechanical parameters used in the calculations and the empirical character of the model, simulations describe the process of solid particle emission from graphite very well. This is evidence that the breaking of bonds between grains due to extremely high thermal stresses is the reason of BD. The mechanism is as follows. Volumetric heating initially results in the thermal expansion of cells and grains, developing thermal stresses in the bonds and, finally, initiates the crack formation in the sample. The cracking of the bonds decreases the heat transfer inside the graphite and increases the temperature of thermally isolated grains. Thermal isolation of one or several graphite grains from the bulk material results in their erosion. Fig. 4 illustrates the temperature as a function of depth in graphite sample after 2ms of power load at 2.4GW m<sup>-2</sup> for RT and 500 °C initial sample temperatures. The temperature distribution has peaks which correspond to thermally isolated grains because of a degradation of the heat transfer and overheating of isolated grains. It is worth mentioning that in the case of pre-heated graphite the amount of thermally isolated grains is higher compared with that for samples loaded at RT. In general, pre-heating reduces the time to reach the threshold temperature



Fig. 2. SEM image (a), experimental cross-section (b) and calculated cross-section (c) of graphite R6650. Absorbed power  $P_{abs} = 2.4 \,\text{GW m}^{-2}$ , pulse duration  $\Delta t = 4.4 \,\text{ms}$ , pre-heated to 500 °C.



Fig. 3. Calculated erosion as a function of time for graphite R6650 pre-heated to 500° C for two values of absorbed power  $P_{\rm abs} = 1.3 \,\rm GW \,m^{-2}$  and  $P_{\rm abs} = 2.4 \,\rm GW \,m^{-2}$ . Experimental data is also shown for comparison.

for brittle destruction (Fig. 5). For this reason, BD starts earlier for the pre-heated samples. The onset of BD,



Fig. 4. Calculated temperature depth profile for absorbed power  $P_{\rm abs} = 2.4 \,\rm GW \,m^{-2}$  and pulse duration  $\Delta t = 2 \,\rm ms$  for graphite R6650 pre-heated to 500 °C and at RT.



Fig. 5. Surface temperature as a function of time for various power loads and initial temperatures.



Fig. 6. Onset of brittle destruction,  $t_{BD}$ , for graphite at room temperature and pre-heated to 500 °C.

which was found from the current reduction during the heat load tests in JUDITH, is shown in Fig. 6. The calculated onset of BD shows a similar decrease for the preheated graphite as for the experimental data. This is a confirmation of the model validity.

### 4. Conclusions

To understand the mechanism of particle emission from carbon based materials during thermal shocks, calculations using the 'PEGASUS-3D' code have been performed. Using the mean failure stress value  $\sigma_{0s} = 0.004$  a good agreement between experiments and calculations for both room (20°C) and high (500°C) initial sample temperatures has been obtained. Calculations show that the influence of different grain size distributions is not significant compared to the mean failure stress. Calculations show similar surface morphology and erosion as experiments for various heat loads and pulse durations. The reason for the enhancement of particle erosion and the reduction of time to initiate the brittle destruction for pre-heated graphite is that the temperature reaches the threshold value for brittle destruction faster compared to unheated samples.

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