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The Evaluation of Deformation and Fracture of Gilsocarbon Graphite Subject to Service Environments: Experimental and Modelling

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Abstract. Commercial graphites are used for a wide range of applications. For example, Gilsocarbon graphite is used within the reactor core of Advanced Gas Cooled Reactors (UK) as a moderator. In service, the mechanical properties of the graphite are changed as a result of neutron irradiation induced defects and porosity arising from radiolytic oxidation. In this paper, we discuss measurements undertaken of mechanical properties at the micro-length-scale for virgin and irradiated material. These data provide the necessary inputs to an experimentally-informed model that predicts the deformation and fracture properties of Gilsocarbon graphite at the centimetre-length-scale. The results provide an improved understanding of how the mechanical properties and fracture characteristics of this type of graphite change as a result of exposure to the service environment.

Introduction

Unlike naturally occurring graphite, commercial graphites are used for a wide range of applications. However, in these cases the graphites usually have complex microstructures and are manufactured to have physical and mechanical properties appropriate to the specific application. An example of this is the Gilsocarbon graphite used in the construction of reactor cores for the civil power-generating UK Advanced Gas Cooled reactors, where properties have been achieved to allow the material to fulfil the structural and neutron moderation requirements. The mechanical behaviour of these reactor core graphites can be described as quasi-brittle [1]. The materials have microstructural features similar to other aggregate-containing materials, such as concrete. Certainly, the nuclear graphite does not exhibit plasticity as it is deformed, so that non-linearity in the load-displacement response is associated with micro-crack formation [1]. As a consequence, a microstructurally-based multi-length-scale finite beam element model is adopted to simulate the mechanical response and fracture characteristics of Gilsocarbon graphite in both the virgin and service-exposed conditions. For the latter, the focus is on simulating the combined contributions of weight loss by radiolytic oxidation and neutron irradiation damage on these properties.

Experimental Measurements

Mechanical properties of virgin and irradiated Gilsocarbon graphite supplied by EdF Energy Ltd were measured. These were undertaken at the appropriate length-scale for input to numerical simulations. It is important to recognise that it is the inherent properties of the material, and not those of the overall microstructure, that are required. These include elastic modulus and fracture strength. For models used in this work, these data are required at the micrometre-scale. Micromechanical properties of this porous nuclear graphite were obtained using a novel technique for testing micro-cantilever specimens. In this approach, small cantilever specimens of the representative material were prepared and tested in a dual-beam work station (FEI Helios NanoLab 600i), which uses an in-situ force measurement system. The cantilevers were milled from regions of

the graphite samples to have cross-sections of $\sim 2\mu m$ and beam lengths of $\sim 10\mu m$, (aspect ratio 5:1). More details about this experimental technique can be found in [2]. The results are summarised in Table 1. These measurements on this length-scale were inputs for the multi-scale computer model.

Condition	Measured area	Young's modulus (GPa)	Bending strength (MPa)
Non-irradiated	Filler particle and matrix	18	564
Irradiated	Filler particle	24	1093
	Matrix	14	330

Table 1. A summary of micro-cantilever test results.

Modelling Approach

Gilsocarbon graphite consists of nearly-spherical filler particles and pores, with complex shapes embedded within the matrix. Microstructural models have been generated for virgin graphite (20% porosity) and to be representative of irradiated graphite (up to 60% porosity). Models of cm cubes with 20% of the volume consisting of filler particles were created (Figure 1), divided into eight 5mm x 5mm x 5mm cubes to match test specimens, with these then subdivided into mm cubes for the multi-scale fracture simulations.



Figure 1. Computer generated microstructure of Gilsocarbon graphite, with filler particles in light grey and large pores in black (20%). Mass loss is simulated by "weakening" the matrix to match the mass loss.

A lattice-type model was used for the deformation and fracture analysis [3,4]. In the model, the material is discretised as a set of small beam elements. A regular cubic grid of beam elements, with equal lengths, is used. A set of linear analyses is then performed by calculating the response of the lattice mesh for a particular external displacement. The beam with the highest stress-to-strength ratio is identified and removed from the lattice network. In each of the analysis steps, a single lattice beam is removed from the mesh, representing the creation of a small crack, and causing a change in the specimen compliance. The analysis is then repeated, with an updated mesh.

To capture the microstructural details of porous graphite, the computational effort necessary for a single-scale approach is too high. Instead, in this study a multi-scale modelling scheme was used. The approach is shown schematically in Figure 2. The multi-scale modelling procedure can be summarised as follows: first, the beam microstructure is divided into a number of small cubes (in this case, each cube was 1mm x 1mm, with a total of 125 cubes); then, a direct tension test is simulated on each of these small cubes (in these simulations, beam elements were assigned brittle behaviour), resulting in load-displacement curves, which are then schematised as multi-linear (Figure 2b). These multi-linear curves for small cubes are used as constitutive relationships for elements in the larger specimen (Figure 2c), which is then tested, resulting in a load-displacement response and cracking patterns for the full-sized specimen (an example is shown in Figure 2d).

In the simulations on the larger scale, the local behaviour of each beam element was, therefore, not brittle. In fact, each element was assigned a multi-linear constitutive relationship which resulted in

simulating the "local" microstructure on the smaller scale. Consequently, on this scale, the beam elements were not removed in each loading step but, for "damaged" elements, the stiffness and strength were adjusted according to their respective constitutive relation.



Figure 2. Multi-scale modelling procedure: (a) a small cube, 20x20x20 voxels; (b) loaddisplacement curve (black), which is the outcome of a small-scale simulation. The grey curve is a schematisation of the black one and is multi-linear, with six segments with points taken at (1) origin, (2) first micro-cracks, (3) peak load, (4) first point in response for which load is <75% of the peak, (5) first point in response for which load is <50% of the peak, (6) first point in response for which load is <25% of the peak, (7) point at which load is zero; (c) detailed mesh shows a small cube (20x20x20 voxels) in grey at its location within the large cube; (d) example load-displacement curve obtained from the full-scale simulation.

Results



Figure 3. Simulated stress strain curves for Gilsocarbon graphite with increasing levels of irradiation damage (legend denotes weight loss).

Porosity levels can be converted to weight loss values, and the change of engineering properties (elastic modulus and strength) caused by combined contributions of radiolytic oxidation and neutron irradiation may be predicted. In Figure 3, simulated stress/strain curves for various weight

loss levels are given, where zero represents the unirradiated condition that contains porosity arising solely from fabrication. A comparison between measured and simulated elastic moduli for increasing weight loss is given in Figure 4. Note that experiments were performed on 6mm x 6mm x 15mm prismatic specimens tested in three-point bending. It can be seen that the predicted values follow the experimentally-measured trend of modulus decrease with increasing weight loss. More work needs to be performed to evaluate the predicted strength values in comparison with experimental data.



Figure 4. Comparison of the simulated (cross) and experimental (circle) values of Young's modulus for increasing weight loss.

Concluding Comments

In this paper, a multi-scale modelling procedure for predicting changes in elastic properties of Gilsocarbon graphite due to service exposure to combined neutron irradiation and radiolytic oxidation is presented. The model is informed by experimental mechanical property measurement using a small-scale approach. This provides the necessary input data at the micro-length-scale. In addition, a microstructural model representative of the Gilsocarbon graphite and the changes affecting it over time has been invoked. Hence, no fitting parameters have been adopted. This makes data collection and property prediction cheap and efficient. The model has the potential to predict changes over the lifetime of AGR graphite cores. Future work will focus on strength considerations.

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