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GLOBAL ENERGY APPROACH TO MODEL CRACK PROPAGATION IN IRRADIATED GRAPHITE COMPONENTS USING NOVEL APPLICATIONS OF THE XFEM FRAMEWORK IN ABAQUS

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ABSTRACT

Modelling crack propagation is a difficult problem, which is compounded for nuclear graphite components by the heterogeneity of the material properties which also evolve with time. The differential rates of dimensional change generate internal stresses that are predicted to become large enough to cause cracks. These may affect the ability of the bricks to perform their structural function and so accurately predicting crack morphologies in irradiated nuclear graphite components enables their consequences for the structural response of the whole core and its safety systems to be evaluated and assessed. The work presented in this paper considers a global energy approach to crack propagation with the aim of understanding, and therefore enabling predictions to be made of, the shapes of the graphite components post fracture. Here, crack propagation has been modelled using facilities within the eXtended Finite Element Method (XFEM) framework in ABAQUS. This has been used to adjust manually the crack propagation directions to maximise the energy release rate. The stability of this propagation can then be assessed by comparing the strain energy release rate with measured values for the work of fracture. The capability of the method is demonstrated by modelling crack propagation in unirradiated graphite components and comparing the resultant crack path with mechanical experiments. Subsequently, the method was applied to predict morphologies and stability of cracks propagating in irradiated graphite bricks.

INTRODUCTION

Fracture in Graphite

Nuclear graphite is a heterogeneous material in which the material properties vary significantly through the component leading to a corresponding variation in fracture behaviour. Moreover, in an advanced gas cooled nuclear reactor (AGR) the material properties evolve as a function of irradiation damage in the form of neutron damage, irradiation temperature and radiolytic oxidation. These cause differential rates of dimensional change leading to internal stresses that are predicted to become large enough to cause cracks and may affect the ability of the graphite bricks to perform their structural function. Such cracks would initiate at the outside of the brick late in life and would only be visible once they had propagated inward to the central bore. It is therefore important to predict how these cracks propagate and whether they can arrest and under what stress conditions. To do this, it is necessary to predict their evolving shapes and the associated changes in energy release rate, and how these change with continued irradiation during operation. This paper presents a method to do this using the eXtended Finite Element Method (XFEM) coupled with a global energy approach.

This paper refers to internal stresses which are used as short hand for residual stresses caused by the differential shrinkage through the thickness of an AGR graphite brick. This nomenclature was used to distinguish between the inherent irradiation behaviour of the graphite brick and the stresses generated by external forces from surrounding components.

Global Energy Criterion

The modelling of crack propagation is significantly dependent on the crack growth criteria, which are used to determine the direction of propagation. An incorrect prediction of crack growth direction leads to unreasonable results. Although the maximum principal stress direction is an obvious candidate it is not universally applicable. For mode I fracture, biaxial tensile stresses around the crack tip/front may occur, which leads to a wrong prediction of the crack path; although this can be improved by increasing the mesh refinement and/or element formulation, it could lead to inefficiencies in the calculation route (Dumstorff and Meschke, 2005)

In Linear Elastic Fracture Mechanics (LEFM), various crack growth criteria require the definition of material specific input parameters. These can yield excellent results, nevertheless in the case where the strength of the component varies through time and position such models possess significant challenges and are considered unsuitable for this application. The J-Integral is commonly used to derive stress intensity factors at the crack tip, which are considered the driving force for crack propagation. However although the J-Integral can be calculated without the requirement of focused meshing, to accurately calculate the J-Integral requires significant mesh refinement around the crack tip and re-meshing each time the crack propagates. This can be computationally expensive and lead to inefficiencies in the calculation route. Furthermore for large structures such as graphite moderator bricks, localised fracture mechanics may neglect the global (away from the crack tip) contributions to crack propagation.

This paper applies a global energy approach where the crack propagation direction is based on a postulate that, from all admissible crack directions which release strain energy, cracks will propagate in the direction that maximises the global strain energy released. There is no check during the XFEM calculations on whether a given crack shape is stable or unstable, so the method does not require the evaluation of stress intensity factors. The evaluation of the crack stability and arrest is done *a posteriori*.

The eXtended Finite Element Method

Preliminary investigations into crack propagation in AGR graphite components used common finite element modelling techniques where cracks propagated along element boundaries. This approach designated the Boundary Condition Method (BCM), modelled propagating cracks in a finite element mesh by progressively separating the elements that lay either side of a pre-defined crack surface. This required the crack path to be coincident with existing element boundaries in the mesh and thus it was necessary to refine at least part of the mesh. Whilst this method allowed for cracks to propagate, it was computationally expensive and significantly laborious. Therefore other finite element methods were explored.

The eXtended Finite Element Method (XFEM) has been established for over ten years. It is a numerical finite element method which allows the study of crack growth along an arbitrary path and does not require the mesh to match the geometry of the discontinuity (Dassault Systèmes, 2012). Cracks are not restricted to element boundaries, allowing for the modelling of complex crack morphologies and eliminating spurious mesh dependency (see Figures 1 and 2).

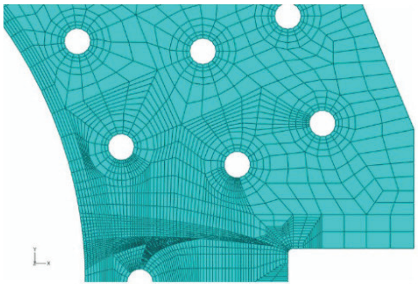


Figure 1 Example of a mesh for conventional FEA crack propagation studies (BCM)

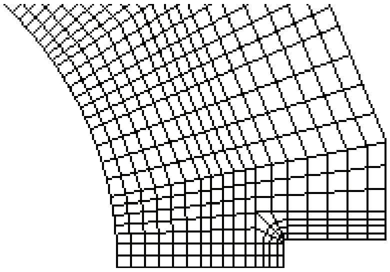


Figure 2 Example of a mesh for XFEM crack propagation studies

In the ABAQUS implementation of XFEM (Dassault Systèmes, 2012), cracks are defined by "shape functions", which describe the crack shape in terms of its position relative to each node of the cracked elements. This process is known as the level set method, a numerical technique for locating and following interfaces and shapes. The values of level sets are known at nodes and interpolated according to the shape functions, being zero at the crack surface/front and non zero elsewhere. Within the general XFEM framework, a crack is defined by a modification to the shape function of cracked elements. The auxiliary level set functions φ and ψ define the position of the crack surface in the element and the plane that perpendicularly intersects the crack front respectively. In ABAQUS these are defined for the crack position relative to each node of the element.

XFEM models cracks by adding degrees-of-freedom to elements in the vicinity of the crack, a process known as "enriching". The additional degrees-of-freedom within the enriched elements allow for the presence of a discontinuity using a special shape function (Giner et al, 2009). There are two types of enrichment implemented in ABAQUS; these are for propagating cracks and stationary cracks, the latter of which includes asymptotic enrichment at the crack front. Propagating cracks automatically grow based on damage criteria and stationary cracks are not permitted to propagate. However, this paper presents a method of adapting the stationary crack method to model crack propagation based on the global energy criterion described above.

ANALYSES

Crack propagation in three dimensions is a complicated concept to model, the propagation of the crack in each of the cardinal (x,y), (x,z) and (y,z) planes has to be considered. Here the problem is simplified by dividing it into two separate processes; two dimensioned propagation using the so called "Fan Trial Method", and three dimension propagation with the "Spline Method".

The Fan Trial Method for 2D propagation

The fan trial method was a trial and error technique developed to predict the preferred direction of crack propagation in two dimensions using the level set method. Various directions of crack propagation were postulated within the confines of an arbitrary cell. The direction that exhibited the greatest release in strain energy per unit extension was considered the preferred crack path. This process was reiterated in subsequent cells until the crack had propagated through the model. For simplicity each cell was restricted to a single element and assumed that the crack extended through the entire cell. This assumption reduced the complexity by only requiring the calculation of the level set defining the position of the crack surface within the element (φ), omitting the level set at the crack tip (ψ). The issue with this assumption was that the crack direction would be sensitive to mesh density and number of fan trials. For this work this assumption was considered an acceptable compromise.

The Spline Method for 3D Propagation

A spline is a curve defined by a mathematical function that connects a series of points in space with a high degree of smoothness. In the context of crack propagation, a spline was used to define the shape of the crack front. Perturbations of the crack front were defined by propagating each point on the spline separately. The preferred direction for crack front extension was determined by the point which exhibited the greatest release in strain energy per unit area. This point was propagated by a user-specified amount which was less than the perturbation size. The other points defining the crack front were propagated as a proportion of the maximum energy release rate for that crack instance. Each instance of the crack was described by level set values calculated within ABAQUS. The spline method provided a means to establish the most energetically favourable path for each crack increment and therefore gave a good description of the crack morphology throughout the propagation.

Mechanical Tests

The two dimensional (2D) work set out to predict the radial crack surface in an irradiation induced stress field using the "fan trial method". The use of the ABAQUS XFEM stationary crack method was validated by modelling crack propagation during mechanical tests (McLachlan et al, 1996) on graphite brick slices that were loaded via the radial keying system as shown in Figure 3.

A range of different crack paths were observed during the mechanical tests. All initiated at the keyway root, the position of maximum stress, but subsequently propagated radially through the brick at a range of angles. The variation was due to the different loading configurations, (i.e. Push vs. Pull) and the variability of strength distributions in the test specimens. Using the fan trial method to propagate cracks based on global energy methods, the stationary crack technique could be validated if it was not constrained to element boundaries and could predict a crack for a pull test where the crack propagated at an angle away from the radial direction, as shown in Figure 4.

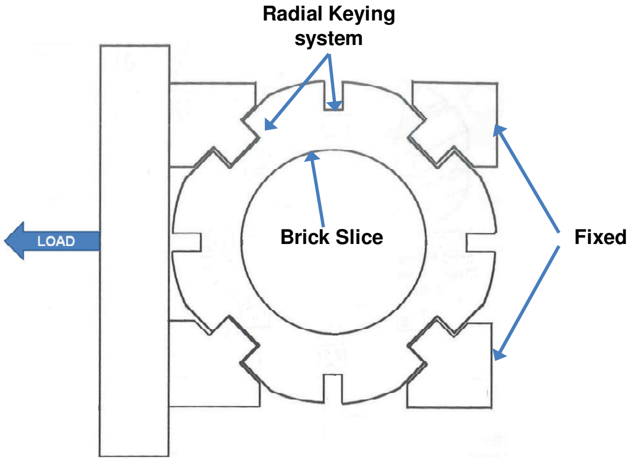


Figure 3 Schematic of the loading set up for the mechanical test with radial key pull loading

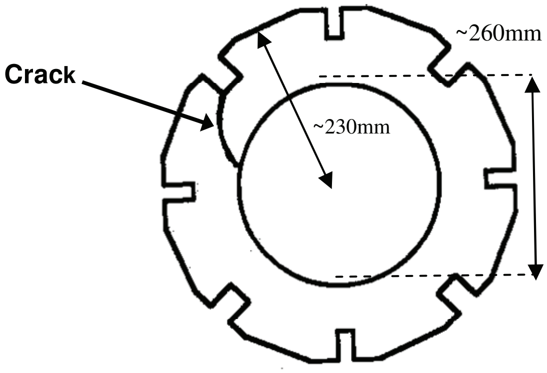
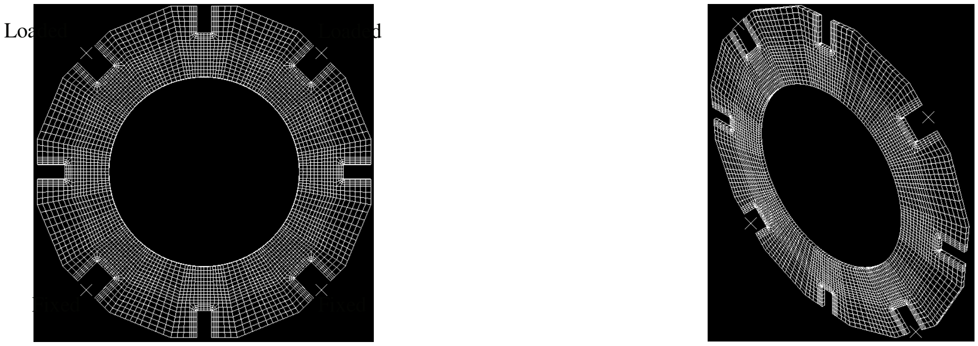


Figure 4 Resultant crack path from the mechanical test with radial key pull loading

Finite Element Models

Note that XFEM stationary cracks in 2D models were not supported in the version of ABAQUS available at the time of this work. Hence 3D models with a single element through thickness were used as quasi-2D models, as shown in Figure 5.



(a) (b)

Figure 5 Finite element mesh for the 2D crack propagation (a) cross-section view (b) isometric view

Generic linear elastic material properties were used for the graphite material with Young's modulus of 10GPa and a Poisson's ratio of 0.2 (Zou et al, 2006). The interstitial keys, which were steel components in the tests, were modelled as rigid surfaces.

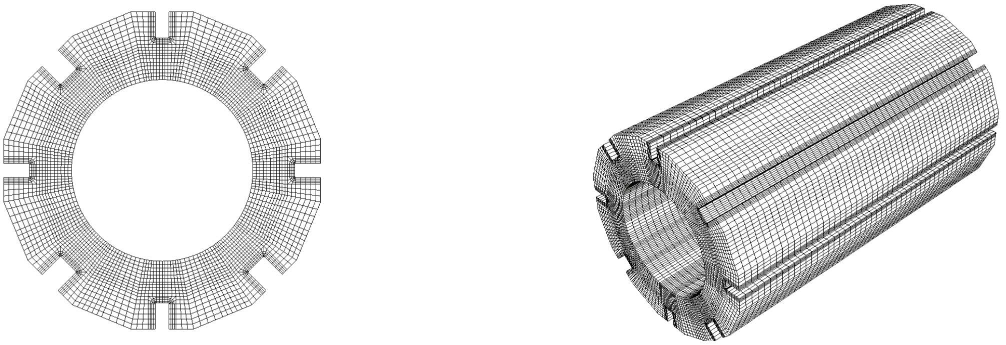
A displacement of 0.625mm was applied to two adjacent interstitial keys in the cardinal x-direction applying a load to the brick slice which was comparable to the failure load of the test specimen (6.2kN). The displacement controlled loading was ramped over a number of increments in one step to simulate the mechanical test conditions for the externally loaded slice case. Fixed boundary conditions were applied to three nodes in the cardinal z-direction which prevented the slice from moving axially. In addition the remaining two interstitial keys were fixed from movement in the x,y and z, to provide a reaction force for the applied load.

Cracks were propagated using the fan trial method and the ABAQUS implementation of XFEM as described above. The crack initiation point was determined by the position of peak maximum principal stress and propagated to the bore. The resultant energy release rate gave an indication of the overall stability of crack propagation. The results from this analysis are described in the results section below.

Irradiation Analyses

The irradiation analyses set out to predict the shape of the crack front and stability of a keyway root initiated crack propagating through an irradiation induced stress field. Due to the complexity of transferring the fan trial method to the 3D models, a new approach using the aforementioned spline method was developed. The methodology of modelling irradiation in graphite fuel bricks is described below:

The finite element mesh used for this investigation is shown in Figure 6. The geometry of the brick is often simplified to keep the model at a manageable size. Unless there is a particular requirement, features such as bore chamfers, methane holes, end face key/keyways may be omitted from the geometry as these do not significantly contribute to the global stresses and deformations of a stand-alone brick (Jones, 2005).



(a) Cross-section view (b) Isometric-View

Figure 6 Views of the geometry and mesh used for the irradiation cases

The mesh used linear reduced-integration 3D continuum elements, ABAQUS type C3D8R (Dassault, systems, 2012), which was a requirement of the XFEM implementation in ABAQUS. To reduce any hour-glass effects, an hour glass stiffness of 22.7MPa was applied to the model.

Deformation of the brick is driven by the neutron damage dose and influenced by the irradiation temperature and weight-loss due to the radiolytic oxidation. Spatial distributions of these field variables through the brick are used to establish the irradiated graphite behaviour.

Stress analyses of graphite irradiation behaviour require many material properties. Some parameters are used directly such as Young’s Modulus or coefficient of thermal expansion (CTE), however other values are used to define the behaviour of the brick, e.g. damage dose and temperature dependencies of properties such as Young’s Modulus, CTE and creep and other coefficients used by the weight loss model. The material models and properties are applied to the stress analyses via the ABAQUS User Material Subroutine (UMAT), which defines the constitutive equations relating the stress and strain in the graphite to the material properties and elastic, thermal and irradiation effects (Jones, 2005).

A full intact (without crack) brick analysis simulating the effects of irradiation from start of life to a time sufficiently late in the core’s operating life was required to generate the internal stress fields due to the degradation mechanisms experienced by the core. It was not possible to propagate a crack using the UMAT hence the stress state was mapped on to another model at a point in the operating lifetime when the tensile stresses in the keyway root were sufficiently large enough for crack initiation to occur. Due to the complexity of transferring the spatially varying distribution of Young’s Modulus onto the cracked brick mesh it was considered appropriate to assume an average value for the whole brick 17.4GPa, and a Poisson’s ratio of 0.2.

Previous work (McLachlan et al, 1996) has shown that internally stressed brick experiments produced cracks which propagated directly to the bore in the radial direction maintaining a single plane. This observation allowed for a simplification in the model, restricting the crack to propagate in the radial and axial direction would restrict the crack propagation to a single plane. This would significantly reduce the complexity of the model. The crack propagation analysis started with a quadrant crack front of radius 10mm that initiated at the bottom of the brick in the keyway root and orientated in the radial straight position. The crack was propagated using the spline method in this plane

Results

Figure 7 shows the resulting crack from the 2D model simulating the mechanical test described above. The crack propagation direction showed that the fan trial method for propagation was not constrained to run along straight lines of elements and was in good agreement with what was observed during the mechanical experiments (shown in Figure 4). In the early stages of propagation, the crack direction changed significantly from the initial path. This could be caused by several factors: the direction of crack propagation in an element was heavily dependent on the element shape; the range of fan trials was not sufficient to capture the actual preferred direction; or the selected initial crack was incorrect. The latter would be the most probable case as substantiated by Figure 8, which shows the energy release rate drops below zero; and therefore the initial crack was not in an energetically favourable position and/or direction.

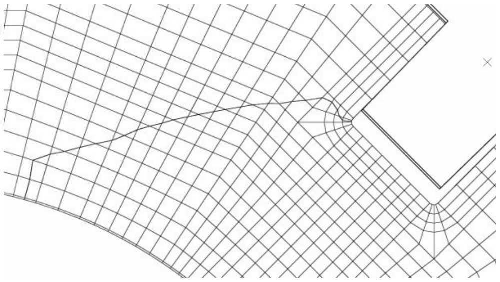


Figure 7 Resultant crack from the model of the mechanical test

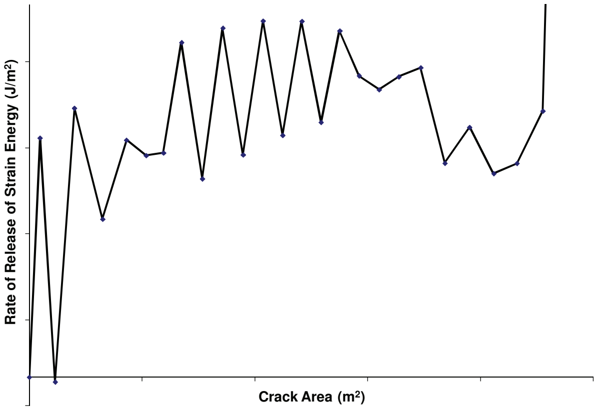
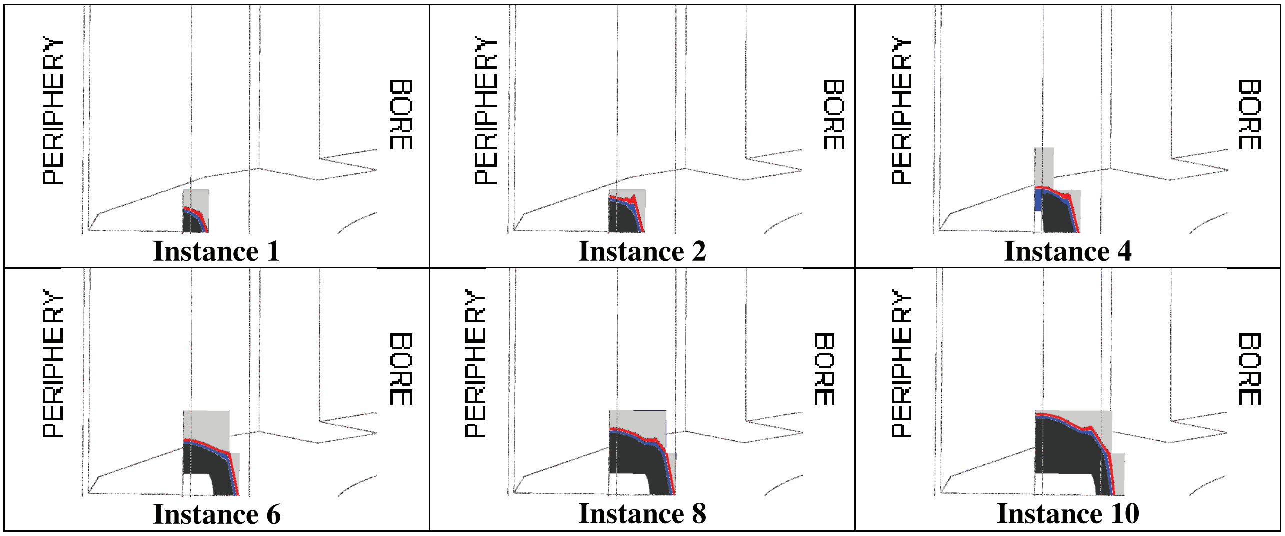
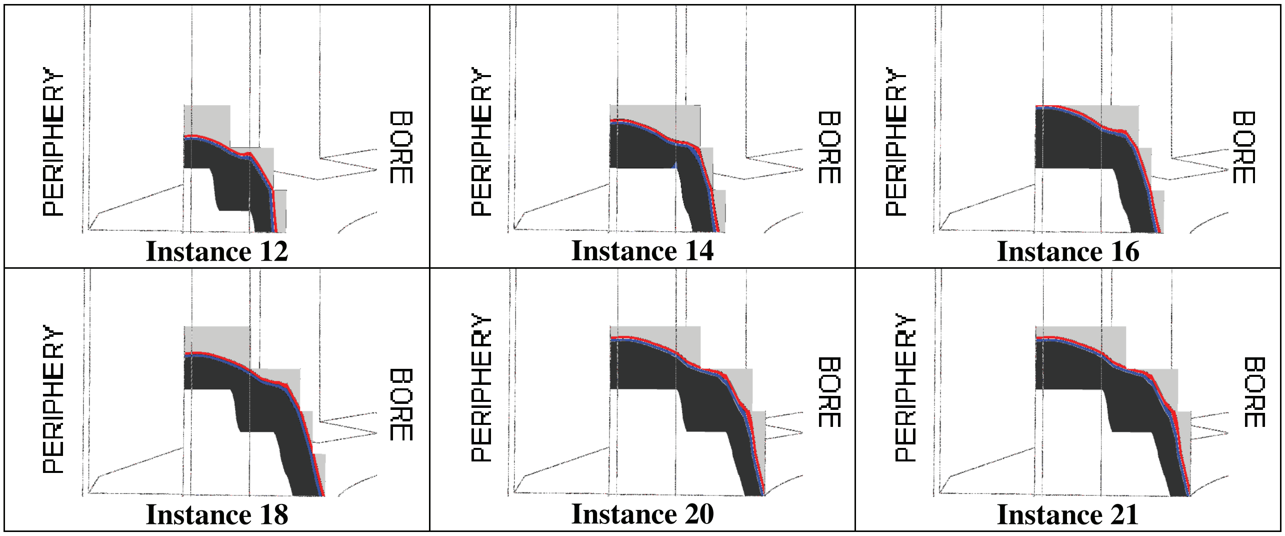


Figure 8 Energy release rate against crack area

Figure 9 shows the resultant crack instances for crack propagation using the spline method in a full 3D brick with irradiation induced stresses. The crack front in these figures is described by the interface between the blue and red contours. Overall the crack front maintained a semi elliptical quadrant shape, albeit with some irregularities attributed to the limited number of perturbation points which defined the crack front. The irregularities could be mitigated by increasing the number of points which define the crack front. However this would increase the number of calculations and would be very labour intensive, (unless the procedure were automated) and was judged unlikely to change the predicted crack front shapes significantly.





Instance 12 | Instance 14 | Instance 16
Instance 18 | Instance 20 | Instance 21

Figure 9 Resultant initial crack instances for a crack propagating in an irradiation induced stress field.

Figure 10 shows the energy released against crack area for the 3D crack propagated using the spline method with irradiation induced stresses. The corresponding energy release rate is shown in Figure 11. The energy released during the initial stages of crack propagation, showed fluctuations of gradient, where the energy release rate alternately increased and decreased. This phenomenon was further demonstrated by the graph of energy release rate; initially there was a lot of noise which corresponded to the changes in gradient in Figure 10. On further investigation, there appeared to be a correlation between the rate of energy released and whether the crack had crossed an element boundary or not. This is most likely an artefact of the mesh and not a real phenomenon, therefore it was considered appropriate to use an averaging technique to smooth the “noise”.

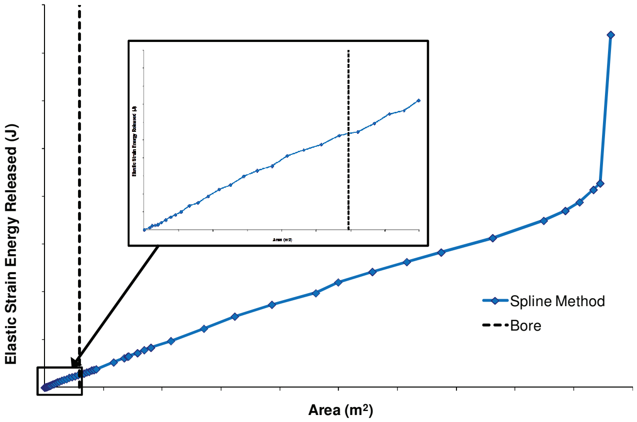


Figure 10 Energy released against crack area in an irradiated stress field using the spline method

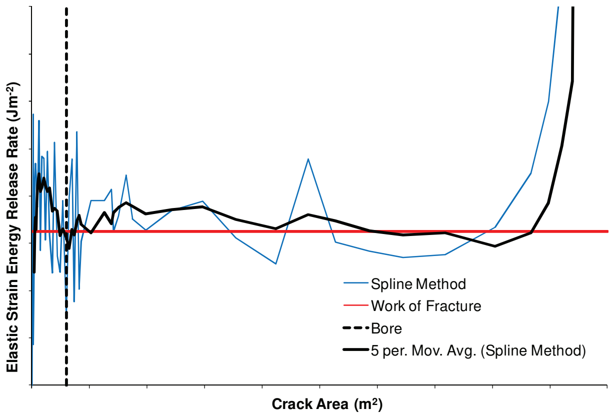


Figure 11 Energy release rate against crack area in an irradiated stress field using the spline method

The “noise” discussed above was reduced by considering a 5 point moving average trend line (plotting the average over 5 points), which is shown by the black solid line in Figure 11. This gave an indication of the underlying trend, which showed a dip following the initial energy release rate before the crack reached the bore and then increased gradually until approximately a third of the crack propagation had occurred where it began to decrease again. The final stage of crack propagation showed a gradual increase in the energy released until the final crack instance and a big release in energy occurred over a relatively small increase in crack surface area.

The stability of crack propagation was difficult to determine without considering the work of fracture of irradiated Gilsocarbon graphite. Unfortunately there was little data available at the time of this work. However it was possible to get an indication of stability by assuming that the energy release rate of the initial crack was greater than or equal to the work of fracture (G_c), indicated in Figure 11 by the red line. If the energy release rate remained above this threshold, the crack would be considered unstable and the crack would continue to propagate. If the energy release rate fell below this value, there was a possibility that the crack could arrest. Figure 11 shows that prior to reaching the bore, the energy release rate due to the propagation of the crack fell below the threshold. By this method we can establish the shapes of stable cracks for a given stress state.

DISCUSSION

The results from the slice test model determined whether the ABAQUS stationary XFEM method could be used to predict crack shapes observed in the experiments. The overall crack shape was in good agreement with the observed behaviour for the brick slice tests with radial key loading. The advantages of using the level set method for predicting crack propagation were that the user has full control of the incremental crack direction and the position of each crack instance is determined relative to the previous propagation. However, the method was very laborious and inefficient which led to difficulties when considering 3D propagation. The fan trial method allowed for a range of discrete crack perturbations within a user defined area (cell) and assessed the preferred direction based on the direction which released the most energy. The user was able to control the complexity of the model by specifying the direction and number of perturbations in each cell.

Although the generic XFEM technique was not mesh dependent in that cracks are not restricted to element boundaries, it was sensitive to the size of crack perturbation and the position of the crack front relative to the underlying element boundaries in the mesh; hence the method adopted, i.e. the fan trial method, limited the crack extent and direction. When considering small crack extents, the releases in energy can be correspondingly small, and when considering the ranges of perturbations, fractions of small amounts were being compared; hence when deciding the most energetically favourable direction, the lack of precision could cause inaccurate results. It would be more appropriate to consider more refined cells comprised of multiple elements, which should give better discrimination of crack directions. Subsequently applied crack front increments could be made smaller to control/refine the morphology of the crack.

The spline method allowed for the modelling of crack propagation in a full 3D brick with irradiation induced stresses. From the results, although each perturbation produced an irregular crack front, the overall shape for each crack instance was reasonably uniform and remained approximately semi-elliptical throughout the propagation. The accuracy of the method could be improved by increasing the number of perturbations/points that described the crack front in each crack instance; however, the technique was very time consuming and an increase in the number of perturbations/points would require a level of automation to increase efficiency.

Analysis of the stability of the propagating 3D crack indicated there was a possibility that a small keyway root crack may arrest and not be visible at the bore; however such a crack would only remain stable until further irradiation caused the stress to increase sufficiently for the energy release rate to exceed the work of fracture after which the crack would become unstable and propagate radially to the bore. Any subsequent arrest would then only occur after significant axial propagation when these cracks would be visible at the bore. Therefore, partially through thickness axial keyway root cracks would only be expected under some limited combinations of circumstances for a short period.

CONCLUSION

This paper presents novel techniques applying the existing extended finite element method in ABAQUS which predicted crack morphologies based on a global strain energy criterion. The ABAQUS stationary crack method coupled with the so called level set and fan trial method was validated by comparing a 2D crack propagation model with experimental tests. The model was extended to 3D by using the spline method to predict crack propagation in an irradiation-induced stress field. Based on the results of this investigation the following conclusions were made:

- Global energy methods coupled with the facilities of the existing XFEM framework in ABAQUS, could be used to predict the stability and shapes of crack growth in nuclear graphite components.
- The level set method and fan trial method are viable techniques for the prediction of propagation in 2D, however the methods would be too labour intensive and inefficient to be applied to 3D propagation without automation.
- The position and direction of the initial crack has a significant impact on the first instances of crack propagation. Accurate representation of the initial defect was important for reasonable results. However, the method would correct the crack trajectory in later stages of crack propagation.
- The 3D models showed significant variation in energy release rate as the crack propagated suggesting that, under some limited combinations of circumstances for short periods, cracks may arrest before reaching either the bore or the far end of the brick.

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