IASMiRT

SMiRT 26
50 Anniversary Berlin/Potsdam

Transactions, **SMiRT-26**
Berlin/Potsdam, Germany, July 10-15, 2022
Division II

FE MODELLING OF SPT SPECIMENS OF IRRADIATED OFE COPPER TO EVALUATE FRACTURE TOUGHNESS USING EXPERIMENTAL DATA

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1. INTRODUCTION

The usefulness of Small-Punch-Test (SPT) specimens to evaluate mechanical properties of materials has gained acceptability over the years. Such tests are particularly suitable in case availability of quantity of materials is very limited or handling of large quantity of materials is hazardous. One of such examples is the irradiated materials in fission and fusion nuclear reactors. Other examples are in-service materials in chemical plants or materials exposed to unhygienic medical and bio industries. Availability of either limited quantity materials or harmful to handle, prevents one to carry out testing of ASTM standard specimens to ascertain change in mechanical properties of materials during in-service operations. However, such data are particularly required to carry out safety studies of plant components and are also mandatory inputs to carry out life extension studies of existing plants.

In the present work, an attempt is made to determine material properties of irradiated OFE copper. These are hardening coefficients n and K of Holloman power law and fracture parameters as a function of irradiation dose. Experimental small punch test (SPT) data reported earlier [1] along with FE modelling are employed for this purpose. FE model consists of conventional elastic-plastic elements and a thin layer of cohesive zone elements along thickness at appropriate location. Such hybrid strategy helped not only to reproduced entire load-displacement curve, but also point of break in the SPT specimens. The material parameters associated with elastic-plastic and traction separation law (TSL) are determined by carrying out parametric studies. The purpose of the parametric studies is to match numerical load-displacement curve with the experimental data of SPT as closely as possible for different irradiation doses including break point. The set of material properties thus obtained are then applied to an ASTM standard TPB specimen. Such numerical approach helped to find out J-initiations and J-R curves of irradiated OFE Copper for various doses of irradiation.

2. EXPERIMENTAL PROGRAM ON IRRADIATED OFE COPPER

Copper and copper alloys are preferred materials in case there are in-service requirements of high electrical and thermal conductivities [2]. Such requirements are more pronounced in case of plasma facing first wall of fusion reactors. Oxygen-free electronic (OFE) grade Copper is one of such materials which have got wide applications, such as, cavity material in Linear Accelerator (LINAC). It is 99.99 % pure as listed in ASTM B 187 Grade C-10100. The chemical composition of OFE copper is given in [3]. An experimental program was pursued earlier to irradiate number of SPT specimens by 10 MeV electrons LINAC for various doses ranging between 11 MGy and 91.5 MGy. The specimens were then tested by using customized die and punch mechanisms. The load-displacement data thus generated were then used to calculate variation in yield stress, ultimate stress, and other associated material properties as a function of dose rate. The load-displacement plots are shown in Fig.1. This work is reported earlier in [1]. While carrying out above work, it was observed that no empirical correlations were available to calculate yield and ultimate stresses of copper alloys using corresponding SPT load-displacement data. To overcome this difficulty, present authors developed new correlations by analysing thirteen different varieties of copper alloys [3].

The SPT load-displacement data shown in Fig.1 are used in the present study to calculate material Holloman power law constants (n and K) as well as cohesive zone TSL parameters [4,5] as a function of irradiation dose. These sets of material properties are then applied to ASTM standard TPB specimen. Such numerical strategy helped to find out J-initiations and J-R curves of irradiated OFE Copper for various doses of irradiation. Details are described in subsequent sections.

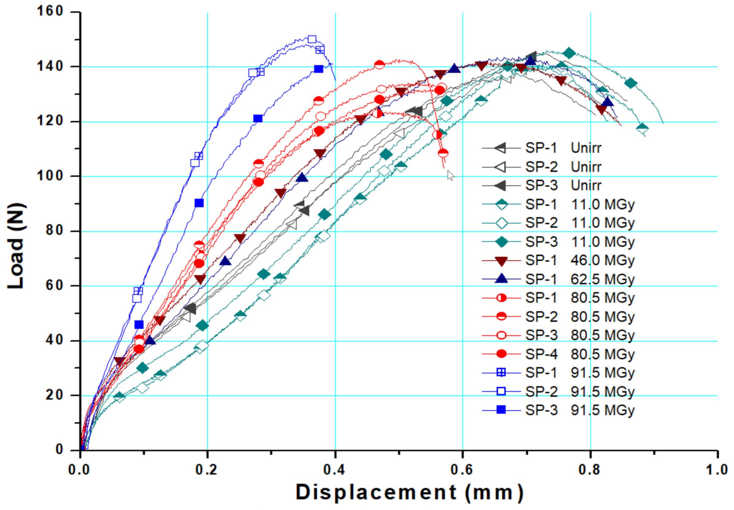


Fig.1 Experimental results of SPT load-displacement data of un-irradiated and irradiated OFE copper SPT specimens [1]

3. FE ELASTIC-PLASTIC ANALYSIS TO ASCERTAIN HOLLOMAN POWER LAW CONSTANTS

3.1 Generation of Material Properties of Un-irradiated OFE Copper

As an extension to the work reported earlier [1,3], present work is carried out to determine Holloman power law constants as a function of irradiation doses to obtain stress-strain curve of irradiated OFE copper. To get a baseline data of Holloman power law constants, three standard tensile specimens of 12.5 mm diameter and 50 mm length of un-irradiated OFE copper are tested. The true stress-strain data thus generated experimentally are used to calculate Holloman power law constants K and n. The Holloman power law which represents the true stress v/s true plastic strain is shown in eq. (3) below.

$$\sigma = \sigma_{YS} + K\varepsilon_p^n \quad (1)$$

Following the conventional methodology, the values of K and n are determined by plotting experimental log $(\sigma - \sigma_{YS})$ v/s log (ε_p^n). The equation of best fit straight line of these data points gives rise to the values of K and n. Table 1 shows the properties of un-irradiated OFE copper thus generated.

Table 1 Mechanical properties of un-irradiated OFE Copper at room temperature

Material	E (MPa)	σ_{YS}(MPa)	σ_{UT}(MPa)	K (MPa)	n
OFE Copper	115000	141	206	317.8	0.159

3.2 Generation of Holloman Power Law Constants of Irradiated OFE Copper

The material property data base shown in Table 1 is then further extended for various values of irradiation doses. For this purpose, the SPT load-displacement curves shown in Fig. 1 are used. The material elastic-plastic properties used in the analysis are represented by Holloman power law. The yield stresses in this equation are taken from [3] as a function of irradiation dose rate. A parametric study is conducted by varying Holloman power law constants with an objective to match numerically calculated load-displacement curve with the experimental results (Fig. 1) as close as possible up to the point of maximum load. The best set of parameters is shown in Table 2 [1]. Figs. 3(a-d) show the numerically calculated SPT load-displacement curves in comparison to experimental results by using various sets of Holloman power law constants including the best set of Table-2.

The following two observations may be drawn from Fig. 3(a), Fig. 3(b) and table 2.

a. Over the range of irradiation doses between 0 MGy to 62.5 MGy, it is possible to get a set of Holloman power law constants which compute SPT load-displacement data close to experimental data. The comparison is reasonably well for the initial shape of the curves as well as maximum loads. This indicates that, there is no significant change in the ductility of the material over this range of doses and elastic-plastic analyses could reproduce the entire load-displacement curves numerically. However, as expected, the elastic-plastic analyses could not indicate the breaking point of the specimens.

b. For the irradiation doses of 80.5 MGy and 91.5 MGy, the parametric elastic-plastic analyses for the best set of Holloman power law constants could not match the numerically calculated load-displacement curves with the experimental data. Over this range, experimentally all the specimens broke much before attending the maximum load. This indicates semi-brittle characteristics of the material for these two doses of irradiation. Such characteristics are also indicated in the variation of yield stresses [3]. In these cases, also, the elastic-plastic analyses could not reproduce the breaking point of the specimens.

Table 2 Best set of mechanical properties determined by parametric studies

	YS, MPa	n	K, MPa
Un-irradiated	141	0.159	317.8
62.5	120	0.15	355
80.5	120	0.1	400
91.5	180	0.05	450

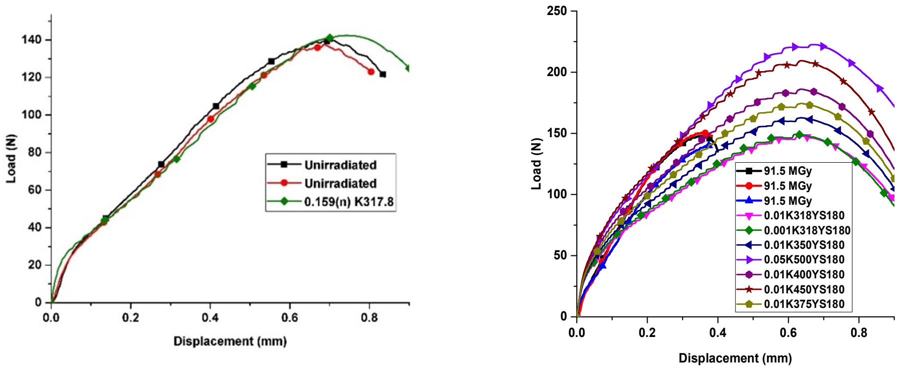


Fig. 3 Results of parametric study to ascertain Holloman Power Law constant for different values of irradiation doses (a) Unirradiated (b) 91.5 MGy

4. ELASTIC-PLASTIC ANALYSIS IN ASSOCIATION WITH COHESIVE ZONE ELEMENTS TO MODEL SEMI-BRITTLE CHARACTERISTIC OF IRRADIATED SPT MATERIAL

As mentioned above, elastic-plastic analyses of SPT specimens unable to reproduce experimental load-displacement data for the specimens which are subjected to cumulative irradiation doses > 62.5MGy. It is primarily due to significant loss of ductility of OFE copper beyond this dose. Experimental breaking loads are found to be much less than the peak loads calculated by elastic-plastic analysis. In addition, elastic-plastic analysis also unable to reproduce the breaking points of the specimens. To overcome these difficulties, a hybrid analysis methodology is presented here. The finite element mesh of the SPT specimen is modified by introducing a thin layer of cohesive zone elements along the thickness. The radial location of this thin layer is appropriately chosen so as to match the breaking location of the specimens as observed during experiment. Fig. 4 shows the updated FE mesh with the location of the cohesive zone elements.

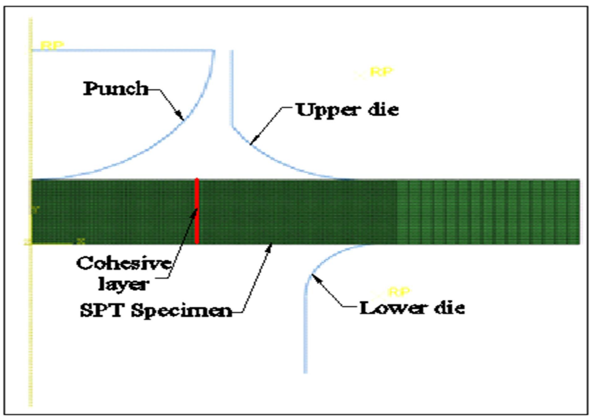
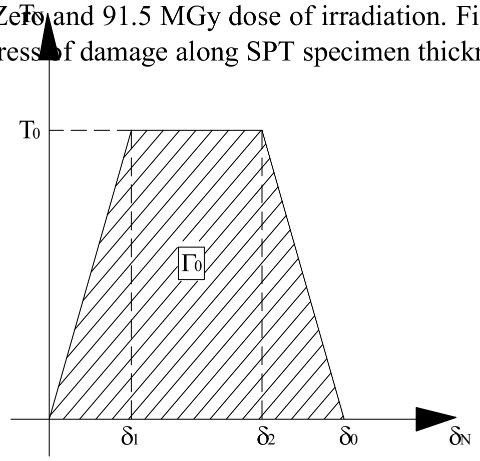


Fig.4 Finite Element mesh of SPT specimen with a layer of cohesive zone elements

The input to the cohesive zone elements is a Traction Separation Law (TSL) [4,5]. In the present study, the shape of the TSL is chosen either bi-linear or trapezoidal depending upon the cumulative irradiation dose of the specimens. Fig. 5(a) shows the shape of the trapezoidal TSL and associated parameters. Fig.

5(b) shows the values of the parameters used in the present analysis for OFE copper. It may be seen that three parameters, viz. Maximum Traction T_0, Damage Ratio "r" [5] and Cohesive Energy Γ_0 are assumed to be varying as a function of irradiation dose. These parameters are subsequently determined by carrying out FE parametric analyses. The parametric studies are carried out to get a best set of these parameters which generates load-displacement data close to the experimental values shown in Fig. 1. Table 3 shows the optimised values of these parameters as a function of doses. It may be seen that for the values of doses up to 62.5 MGy, the 'r' parameter is found to be negligible, signifying suitability of bi-linear TSL for these cases. However, for higher values of doses, i.e., 80.5 MGy and 91.5 MGy, parameter 'r' is found to be non-zero, signifying suitability of trapezoidal TSL for this range of doses. Such change in shape of TSL is expected to be due to significant loss of ductility of OFE copper for higher range of irradiation doses and material behaves like semi brittle material. Figs. 6(a) show the comparison of experimental load-displacement data with the results of FE analysis using cohesive zone elements for OFE copper subjected to Zero and 91.5 MGy dose of irradiation. Figs. 6(b) show the applied TSL for these cases. Fig 7 shows progress of damage along SPT specimen thickness during FE analysis leading to fracture.



Young's Modulus E=115000MPa

Poisson's Ratio=0.31

Friction factor=0.2

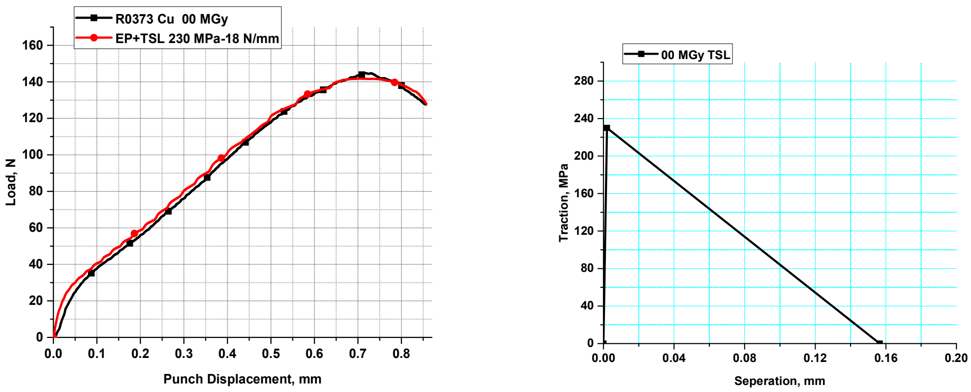
$T_0/\delta_1=E_{nn}=E_{ss}=E_{tt}$ = 115000MPa

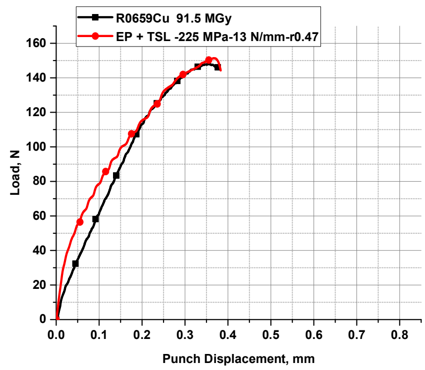
T_0 (Maximum Traction): Varying

$r=(\delta_2-\delta_1)/\delta_0$: Varying

Cohesive Energy (Γ_0): Varying

Fig.5 (a) Description of trapezoidal TSL and associated parameters and (b) Values used in the present analysis





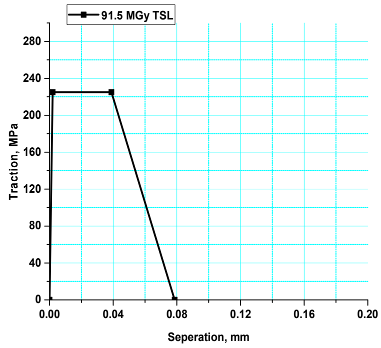


Fig. 6 Comparison of experimental load-displacement data with FE results along with cohesive zone elements and plots of TSL of cohesive zone elements for un-irradiated and 91.5 MGy irradiation doses

Table 3 Holloman power law constants and TSL parameters

Irradiation data	Holloman power law constants			Cohesive zone TSL parameters		
	n	K (MPa)	YS (MPa)	T_{max} (MPa)	Fracture Energy (N/mm)	r
Un-irradiated	0.159	317.8	141	230	18	0
62.5 MGy	0.15	355	120	248	15.2	0
80.5 MGy	0.1	400	120	268	15	0.2
91.5 MGy	0.05	450	180	225	13	0.47

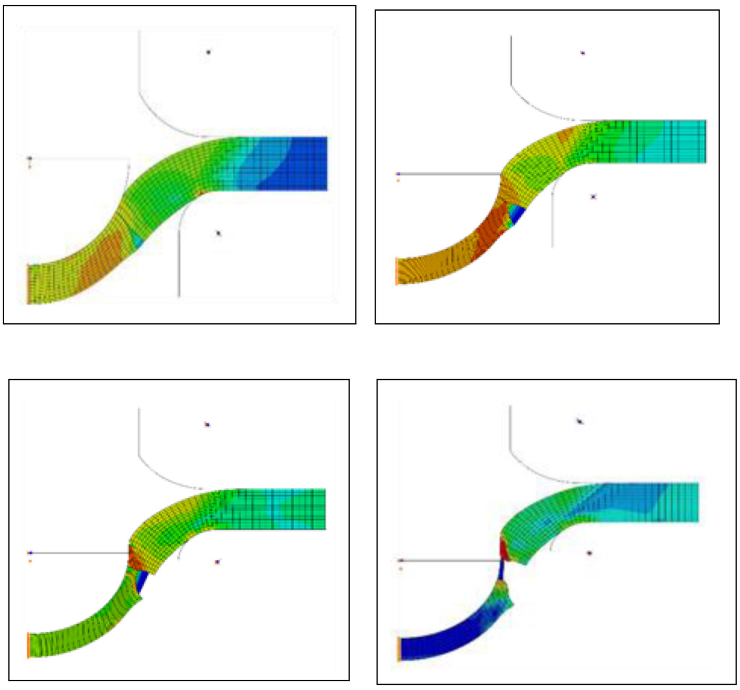


Fig. 7 FE analysis of SPT specimen with cohesive zone elements: typical progress of damage along specimen thickness leading to fracture

5. ANALYTICAL PREDICTION OF FRACTURE TOUGHNESS OF IRRADIATED OFE COPPER

The material parameters shown in Table 3 above are subsequently used to assess fracture toughness of irradiated OFE copper as a function of irradiation dose. For this purpose, FE model of an ASTM standard TPB specimen is prepared. Schematic diagram of the specimen is shown in Fig. 8 (a). The dimensions of the specimen are 112.86x6.76x25.08 mm (LxBxW) and initial crack length is 7.6494 mm, which makes a_0/w as 0.3. The FE model is shown in Fig. 8 (b). The 4-noded 2-D plane strain iso-parametric elements with appropriate boundary conditions are used in the model. Cohesive zone elements are placed partially along the remaining ligament of the specimen in front of crack tip. Such modelling strategy enables to model crack propagation by carrying out elastic-plastic analysis of the TPB specimen in association with cohesive zone elements.

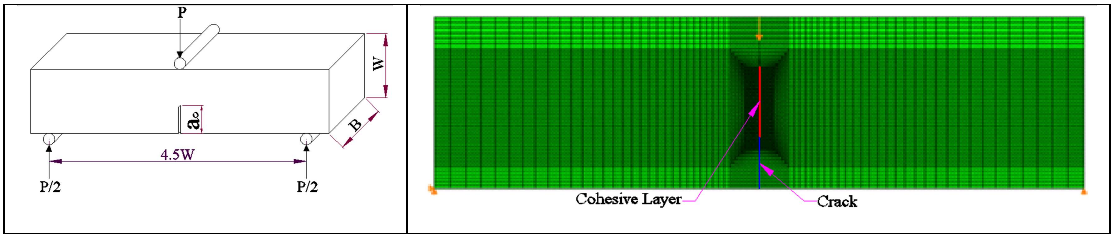


Fig. 8(a) Schematic diagram of a TPB specimen used in the present analysis, (b) FE model of TPB specimen showing the crack and location of cohesive elements along crack line

The analyses are carried out separately for different dose of irradiation, viz. un-irradiated, 62.5 MGy, 80.5 MGy and 91.5 MGy. The elastic-plastic material properties and TSL parameters shown in Table-3 are used. The output of FE analysis is load v/s CMOD and crack growth v/s CMOD data. These data are then converted to J-integrals as a function of CMOD using the procedure described in ASTM 1820. Fig. 9 shows J-integral as a function of crack growth for different values of irradiation doses. It may be seen that the material J-initiation and ductility decreases with the increase in irradiation dose. Fig. 10 shows the variation of J-initiation as a function of doses. Following linear equations may be used to interpolate J-initiation for intermediate values of irradiation doses Φ derived from Fig. 9.

$$\text{J-initiation} = 30.92 - 0.0840\Phi \qquad 00.0 \leq \Phi \leq 62.5$$

$$\text{J-initiation} = 25.67 - 0.2917\Phi \qquad 62.5 \leq \Phi \leq 80.5$$

$$\text{J-initiation} = 20.42 - 0.6072\Phi \qquad 80.5 \leq \Phi \leq 91.5$$

Here J-initiation is in N/mm and irradiation dose Φ is in MGy. A comparison of J-initiation of un-irradiated OFE copper calculated in the present work with the values quoted in literature is shown in Table 5.

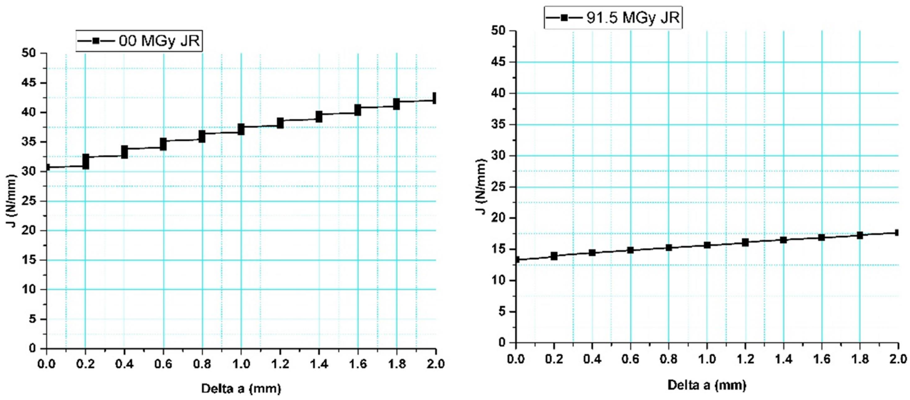


Fig.9 J-R Curves for un-irradiated, 62.5 MGy, 80.5 MGy and 91.5 MGy of irradiation doses

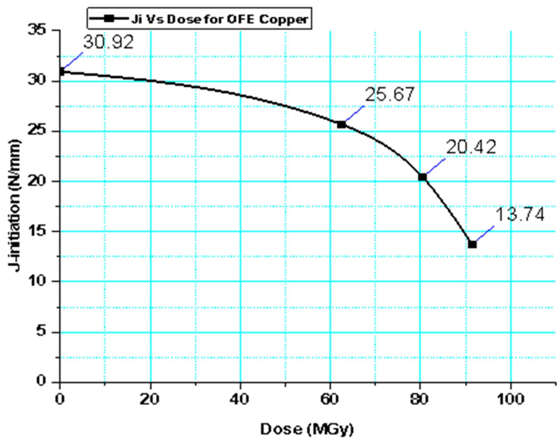


Fig.10 Variation of J-initiation with irradiation dose

Table 5 Comparison of J-initiation of un-irradiated OFE copper calculated in the present work with the values quoted in literature

Material	J-initiation calculated in the present work (N/mm)	Erlangen, FAU University Press (2018) **[6]**	OZAM **[7]**	Altenberger, et. all. (2015) **[8]**
Un-irradiated OFE Copper	30.92 N/mm	29.28 N/mm (60 MPa√m)	12.6 –78.6 N/mm (40-100 MPa√m)	52.85 N/mm (82 MPa√m)

6. CONCLUSIONS

Following conclusions may be drawn from the present work.

a. A methodology has been presented to utilize SPT results to calculate fracture toughness of the material.

b. The steps to calculate fracture toughness are as follows.

    i. Calculate yield and ultimate stresses employing existing correlations using SPT load-displacement data.

    ii. Ascertain Holloman power law constants (K and n) by carrying out parametric studies with an objective to match FE load-displacement data with the SPT results between yield loads to ultimate loads.

    iii. Determine TSL parameters of cohesive zone by carrying out parametric studies with an objective to match SPT data between ultimate load and breaking point by carrying out elastic-plastic analysis of FE-CZ hybrid model.

    iv. Calculate J-initiation and J-R curve of the material by carrying out FE-CZ analysis of an ASTM standard TPB specimen utilizing Holloman power law constants and TSL parameters determined in steps (ii) and (iii) respectively.

c. Above methodology is used to obtain J-initiation and J-R curve of OFE un-irradiated copper by carrying out small-punch-tests and FE-CZ hybrid numerical analysis. The calculated J-initiation is in reasonable agreement with the quoted value in the literature.

d. After validating, the methodology is used to calculate J-initiation and J-R curve of irradiated OFE copper for different doses of irradiation.

e. It is found that the fracture toughness of OFE copper decreases rapidly for higher values of irradiation doses beyond 62.5 MGy. This phenomenon is also manifested by the variation of yield stress with the irradiation dose reported earlier [1].

f. The J-initiation of un-irradiated copper calculated in the present work is found to be lying within the quoted values of the literature, despite having large scatter in the literature values.

g. It is expected that the variation of J-initiation and J-R curves with irradiation doses quantified for OFE copper will be useful information for the designers of components made up of this material.

h. The methodology described here to calculate J-initiation and J-R curve using SPT results will be useful information to active researchers in this area.

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