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COUPLED MACROSCALE-MICROSCALE MODEL FOR HYDROGEN EMBRITTLEMENT IN POLYCRYSTALLINE MATERIALS

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ABSTRACT

Prediction of hydrogen embrittlement within a component requires the influence of several length scales to be accounted for. The loads that affect the rate of hydrogen diffusion, typically thermal and structural, derive from the macro or component scale. Micro-structural analysis has an important role to play in providing accurate estimates of the typically homogenous material characteristics employed at the component scale. This contribution considers the coupling of a micro-scale model with the component scale. A micro-scale model is employed in critical regions of the component where resolution of the heterogeneous behavior is necessary. A tie boundary/cut boundary technique is introduced to couple the micro-scale model to the macro-scale model. The developed technique offers a computationally efficient procedure to analyze the multi-scale inter-granular hydrogen embrittlement in a polycrystalline material. This work is targeted at the prediction of hydrogen embrittlement in pulse-plated nickel and is carried out within the context of the EU FP7 MultiHy project.

Keywords: Hydrogen Embrittlement; Multiscale modelling; Hydrogen diffusion; Cracks; tie boundary/cut boundary technique; micro-macro-scale-model.

INTRODUCTION

Hydrogen embrittlement often plays an important role in the catastrophic failure or premature brittle rupture of a structural component. Prediction of hydrogen embrittlement phenomena within a component requires multiple length scales to be accounted for and has attracted research attention over a significant period (Frankel and Latanision [1], Song and Curtin [2] and Jothi et al [11-12]). Some mechanisms that affect hydrogen embrittlement include hydrogen diffusion in short circuit paths such as grain boundaries (Palumbo *et al.* [3],

Watanabe [4] and Gertsman *et al.* [5]) and triple junctions (Gertsman [6]). Intergranular mechanisms such as segregation of hydrogen and hydrogen traps along grain boundaries and triple junctions affect hydrogen embrittlement in the form of intergranular embrittlement (Palumbo *et al.* [7] and Latanision and Opperhauser Jr. [8]). The hydrogen embrittlement mechanisms of cracking are intrinsically microstructural level and have frequently been regarded as microstructural intergranular phenomena (Yao and Cahoon [9], MacCallum and Levine [10] and Jothi *et al.* [11]). So it is important to include these microstructural intergranular phenomena at the design stage to investigate the hydrogen embrittlement mechanisms and life prediction analyses of structural materials at the component level. Computational investigation of the component macro-scale hydrogen embrittlement problem, including detailed heterogeneous microstructure, usually requires the use of supercomputers. In practice, to avoid this complexity the component macro-scale hydrogen embrittlement problem is investigated by neglecting the detail of the microstructure of the polycrystalline material. But such component level macro-scale models provide limited understanding of the hydrogen embrittlement problem. In this contribution a multiscale modeling technique is proposed which accounts for the effects of the heterogeneous microstructure in an investigation of the hydrogen embrittlement phenomena at the component level.

The proposed multiscale model is capable of resolving the necessary microstructural phenomena simultaneously with the continuum degrees of freedom with less usage of computer resources and decreased computational time. In this paper such a method is described; coupled microstructural and continuum including critical defect site (CMCD) modeling method using substructural and submodelling technique to investigate the hydrogen embrittlement mechanism. The CMCD technique consists of a microstructural model (micro scale) near critical sites such as cracks, defects and voids as a substructure or a submodel coupled to continuum models (macro-scale) away from critical sites. The CMCD method thus replaces the continuum domain near the critical sites by including the microstructural phenomena such as grain, grain boundaries, triple junction, voids, defects and clustered grains within the model.

COMPUTATION METHODOLOGY OF CMCD TECHNIQUE

The component level macroscopic body is considered as macro continuum domain (Ω_c) and modeled as global continuum model with single or multiple pre-existing critical microcrack sites or without any pre-existing microcrack. The micro domain near the critical defect site is

modeled as intergranular and intragranular heterogeneous microstructural model by implementing the required microstructural phenomena. In the micro domain (Ω_m) region any microstructural defects such as voids, triple junctions, traps sites, amorphous regions, grain boundaries, clustered grains and dislocations may be considered dependent upon the nature of the problem. Details of the model of the micro domain with heterogeneous two phase intragranular and intergranular microstructural model can be found in Jothi *et al.* [11-12]. In the case of an initially continuum model without pre-existing defect sites, the analysis is run to find the critical defect sites in the continuum model. These critical sites are then modeled as micro domains.

The CMCD modeling technique can be employed using two methods to couple the micro domain to the continuum domain as illustrated in the Figure 1. These alternative approaches are the (i) substructure micro domains (Ω_{mss}) method and (ii) submodel micro domain (Ω_{msm}) method. The substructure micro domain (Ω_{mss}) is coupled through a tie boundary ($\partial\Omega_t$) with the continuum domain (Ω_c) and then the boundary value problem is solved as one single problem. The submodel micro domain (Ω_{msm}) is coupled as cut boundary ($\partial\Omega_c$) with the continuum domain and then the boundary value problem being solved as two decomposed problem as shown in Figure 1(d). The detailed information about cut boundary and tie boundary methods can be found elsewhere [13, 20-21]. In brief, these boundary techniques allow the creation of refined element meshes in the localized micro submodel/substructure regions with the same degree of freedom as the global macro model. The localized micro submodel reacts to the load and boundary conditions of the global macro model. The tie and cut boundary elements and nodal DOFs, load and boundary condition datasets are stored in a different data file and is handled using subroutine programs to run the localized micro submodel/substructure analyses.

As a test, the proposed CMCD technique is implemented to investigate the hydrogen embrittlement mechanism. The present model will connect the hydrogen diffusion and accumulation mechanism in the microstructural region to macroscopic hydrogen embrittlement. The model includes the heterogeneous intragranular and intergranular microstructural defects as a substructure or submodel near critical sites. This localization of the microstructural domain limits the expenditure of computational resources and allows much more detailed information to be obtained for the embrittling effects of hydrogen in structural polycrystalline materials. The features of this CMCD technique are that the critical microstructural defect sites are present in the continuum model and

coupled in the form of heterogeneous intragranular and intergranular microstructure. The information from continuum domain can be passed to the microstructural Ω_{mss} or Ω_{msm} so that the hydrogen embrittlement mechanism can be investigated at the microstructural level and understood better with detailed microstructural information.

The hydrogen diffusion boundary value problem for this CMCD model is solved using finite element method by employing the *weighted residual Galerkin method* developed within the finite element analysis software ABAQUS. PYTHON script has been developed to link the macro-micro models in the form of boundary techniques. This work tests the two methods of the CMCD modeling technique by investigating the hydrogen embrittlement mechanism using hydrogen diffusion problem based on Fick's law using two methods, initially with substructure micro domains (Ω_{mss}) method and then with a submodel micro domain (Ω_{msm}) method. Both the problems modeled are limited to traps, stress and strain assisted diffusion. Figure 2 shows the schematics of the CMCD modeling technique.

HYDROGEN DIFFUSION LAWS

The CMCD modeling technique is initially implemented for the flux of hydrogen atoms i.e. diffusion of hydrogen as described by Fick's laws from the high concentration regions to low concentration regions. The hydrogen flux vector J_c consists of a hydrogen concentration gradient ∇C at a specific time t based on *Fick's first diffusion law* by using the *thermodynamic formulation* based on the *Gibbs free enthalpy*. The CMCD model consists of a macro domain continuum model Ω_c and micro domain Ω_m microstructural model. The micro domain microstructural model consists of a representation of two phases, intergranular and intragranular. These phases are assigned separate material properties, for example the intragranular hydrogen diffusion coefficient D_{ig} and the intergranular hydrogen diffusion coefficient D_{gb} . The modeling procedure for the micro domain is explained in detailed in Jothi *et al.* [12]. The macro domain continuum model is modeled with the effective hydrogen diffusion coefficient D_{eff} which is the combination of D_{ig} , D_{gb} , and its calculation is shown in Jothi *et al.* [12]. The Arrhenius form of diffusion coefficient can be described as $D_0 \exp(-E/RT)$, where E is the activation energy, T is the absolute temperature, R is the ideal gas constant, C is the concentration of hydrogen, the gradient operator is represented by ∇ , Laplace operator is Δ and X represents three dimensional position.

$$J_c(X, t) = -D_{eff} \nabla C(X, t) \quad (1)$$

The commercial software ABAQUS implements the above diffusion equation as shown in equation (2)

$$J_C(X,t) = -sD_{eff} \nabla \phi(X,t) \quad (2)$$

Where s is the solubility of the material and $\phi = C/s$ is the normalized hydrogen concentration.

Based on the *law of matter conservation*, the amount of hydrogen is expressed by the continuity equation based on a transient (time dependent) diffusion process as described by *Fick's second law*

$$\frac{\partial C}{\partial t} = -\text{div } J_C \quad (3)$$

$$\frac{\partial C}{\partial t} = D_{eff} \nabla^2 C = D_{eff} \Delta C \quad (4)$$

The implementation of the governing diffusion equation in ABAQUS is shown in equation (5) and further information can be found elsewhere [11-13, 15-21]

$$\frac{\partial C}{\partial t} = s D_{eff} \Delta \phi \quad (5)$$

NUMERICAL ANALYSIS PROBLEM STATEMENT OF CMCD MODEL WITHOUT AND WITH CRACK

The present CMCD model is tested by simulating hydrogen diffusion in two example problems on a two dimensional system. The initial problem is without any cracks and the second one includes a single microcrack in the form of sharp notch in the round test piece. The geometry and boundary conditions for hydrogen entry are sketched in Figure 3 and Figure 4 respectively for each of the models. Figure 3 and Figure 4 show the CMCD model micro domains embedded within continuum macro domain, without a crack and with a crack respectively. Note all the material properties used in the analysis are given in the appropriate figure captions. Figures 3(a) & (b) show the space shuttle launcher thrust chamber geometry on the metre scale and in close-up view respectively. Figure 3 (c) shows the close-up view of the thrust chamber macro domain cross section coupled to the micro domain.

In the CMCD without a crack model, the coupled micro domain using a tie boundary with the homogenised continuum domain is shown in Figure 3(d). The area of the micro domain is $36\mu\text{m}^2$ and the average grain size is $6\mu\text{m}$. Figure 3(e) shows the boundary conditions for hydrogen entry into the surface of the material as an environmentally

controlled concentration of hydrogen. Figure 3(f) shows the tie boundary (in yellow) coupling the macro and micro domains of CMCD model. The reader should refer to the respective figures for the diffusion property values used in the models. In the CMCD with a crack model, the micro domain is confined to a small domain in the critical region near the corner of notch in the test piece. The remaining region is considered as a homogenized continuum domain as shown in Figure 4(a). Cortés *et al.* [14] consider the three dimensional round sharp notch test piece as a two dimensional axisymmetric model to analysis the hydrogen embrittlement problem by examining the effect of a crack starting from the root of the sharp notch. The two dimensional sharp notch geometry considered here is used to test the hydrogen transport mechanism of the CMCD model with a crack (i.e. the sharp notch is considered as a crack as shown in Figure 4 (a)). Figure 4 (b) shows the axisymmetric boundary condition and the boundary condition of hydrogen concentration entering into the surface of the structural polycrystalline material. Figure 4 (c) shows the coupling of the micro domain and homogenised continuum domain via the tie boundary. The mesh used for the CMCD model without a crack and with a crack and the close-up view of the meshed micro domain region are shown in Figures 5 and Figure 6 respectively.

The simulation of the CMCD model with a crack and the CMCD model without a crack has been performed to investigate the hydrogen embrittlement mechanism of a polycrystalline material using a two dimensional hydrogen diffusion simulation. Figure 5 shows contours of the hydrogen concentration within the intragranular and intergranular heterogeneous microstructure in the CMCD without a crack model where the subscale micro domain and the homogenous behaviour of the hydrogen diffusion mechanism at the macro scale continuum level are solved using a substructure micro domain method. In order to validate the developed CMCD model with both tie boundary and cut boundary technique, initially the hydrogen diffusion analysis has been done using single diffusion property in both micro and macro domain as well in intergranular and intragranular domain. The diffusivity used in the model is $2 \times 10^{-12} \text{ m}^2/\text{s}$. The results of this analysis are shown in figure 5 (a) on three various elapsed time 20s, 60s and 400s. In order to validate the developed CMCD model with both tie boundary and cut boundary technique, a preliminary hydrogen diffusion analysis has been done using a single diffusivity in both micro and macro domains as well as in the intergranular and intragranular domains. The diffusivity used was $2 \times 10^{-12} \text{ m}^2/\text{s}$. The results of this analysis are shown in figure 5 (a) for elapsed times of 20s, 60s and 400s. In order to validate the CMCD model based on tie and cut boundary techniques, the hydrogen diffusion analysis results are plotted for three different positions X1, X2 and X3 (i.e. in the

cross section of the outer nickel layer of the thrust chamber from outer surface to inner surface at distances of $X_1=7\mu\text{m}$, $X_2=8\mu\text{m}$ and $X_3=11\mu\text{m}$) in both micro domain and macro domain of thrust chamber outer nickel layer cross section. These plots are shown in the figure 5 (b). The tie and cut boundary micro domain results are in good agreement with the macro domain results.

Two test cases were analysed using the CMCD model without a crack model using different diffusion properties in the micro domain and macro domain to show the effective application of the techniques. The homogenous effective diffusivity (i.e. the diffusivity used in the macro domain is $2 \times 10^{-12} \text{ m}^2/\text{s}$. (Note: A finite element microstructural homogenization technique has been used to calculate the effective diffusivity for an average grain size of $1\mu\text{m}$ and detailed description of this can be found elsewhere [12, 20-21].) An averaged grain size of $1\mu\text{m}$ has been used in macro domain with different diffusion properties in grains and grain boundaries in the micro domain (diffusivities used in the intragranular region and intergranular regions are $9 \times 10^{-14} \text{ m}^2/\text{s}$ and $4 \times 10^{-10} \text{ m}^2/\text{s}$ respectively). Figure 5 (c) shows the results of the CMCD model without a crack using the tie boundary technique and figure 5 (d) shows the results of the CMCD model without a crack using the cut boundary technique.

In order to show the application of CMCD model in the cracked domain another test case has been analysed with a crack using the CMCD model and boundary techniques. The hydrogen diffusivities used in the macro domain is $1 \times 10^{-13} \text{ m}^2/\text{s}$, in the micro domain the diffusivities used in the intragranular region and intergranular region are $9 \times 10^{-14} \text{ m}^2/\text{s}$ and $4 \times 10^{-10} \text{ m}^2/\text{s}$ respectively. Figure 6 shows the equivalent plots for the test case of the CMCD model which includes the crack. Figure 7 shows the resolved hydrogen concentration and accumulation for the intergranular and intragranular microstructural micro domains at various elapsed times (i.e. $t_1=2.29 \times 10^5 \text{ s}$, $t_2=4.9 \times 10^5 \text{ s}$, $t_3=1.13 \times 10^6 \text{ s}$, $t_4=4.1 \times 10^6 \text{ s}$, $t_5=6.1 \times 10^6 \text{ s}$, $t_6=1 \times 10^7 \text{ s}$) for the CMCD crack model based on a substructure micro domain method. This simulation shows detailed information about the modelled hydrogen diffusion, aggregation and accumulation in the heterogeneous polycrystalline structural material.

The predicted hydrogen concentrations obtained through representing the micro scale intragranular and intergranular geometry and physics within the current model demonstrates how they play an important role in the aggregation of hydrogen concentration near critical sites and interfacial areas. These critical and interfacial areas

accumulate hydrogen more than elsewhere. This detailed local microstructural interfacial information about the hydrogen diffusion, accumulation, and aggregation gives a better understanding about the intergranular hydrogen transport mechanism. The model also has the potential to study and understand the crack nucleation, propagation, critical hydrogen concentration and debonding of materials along the interfacial critical region of a structural polycrystalline material.

The proposed multi scale CMCD model couples the microscopic details to the macroscopic region using tie boundary and cut boundary techniques. It can be used for modeling the location of critical sites providing more detailed information. The incorporation of microstructural details into the macroscopic continuum region may help to predict hydrogen embrittlement at the design stage providing a better understanding of hydrogen diffusion phenomena and much more detailed local microstructural information of the hydrogen transport.

CONCLUSION

In summary we have proposed a technique to analyse the hydrogen embrittlement of polycrystalline material that couples the component level macroscopic region with the microstructural region. In the microstructural region, the two phase heterogeneous microstructures, the intragranular and the intergranular, are geometrically represented. This is a true two scale CMCD technique which enables the investigation of the hydrogen embrittlement phenomena of heterogeneous polycrystalline materials by treating it as a single micro-macro critical domain, multiple micro-macro critical domains or multiphase heterogeneous micro-macro domains including voids, defects, triple junctions and traps. These models also provide a route to do further coupled multiscale modelling by coupling the micro-meso-macro domains depending on the nature of the problem. Other key strengths of the present modelling technique are the usage of less computation resources and a decrease in computational run time.

The present modelling technique seems to be a promising multiscale tool that could be used in the design stage for life prediction in polycrystalline structural materials. It could also be used to provide a qualitative understanding of the role of a large number of hydrogen embrittlement phenomena such as hydrogen diffusion, aggregation, accumulation mechanisms in the microstructure and at the continuum scale. The models have the potential to study premature brittle rupture or catastrophic intergranular hydrogen embrittlement

problems that cannot easily be treated by either fully microstructural models or existing macrostructural models.

The present CMCD technique can be extended to implement stress assisted hydrogen diffusion, strain assisted hydrogen diffusion, hydrogen traps, triple junctions, grain orientation, clustered grains, voids and defects. Other applications such as coupling the atomistic model will be the subject of future work.

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FIGURES

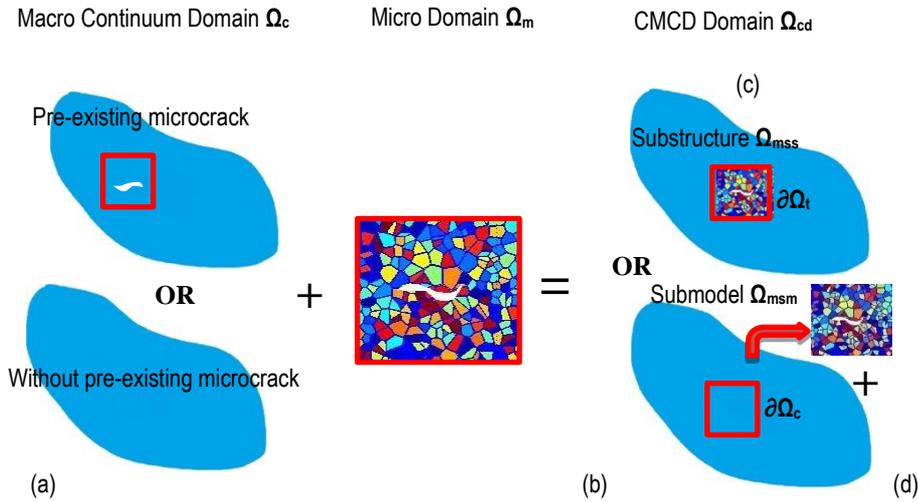


FIGURE: 1- Schematic of the coupled microstructural and continuum critical dislocation site model using heterogeneous intragranular and intergranular microstructural domain as substructure or submodel.

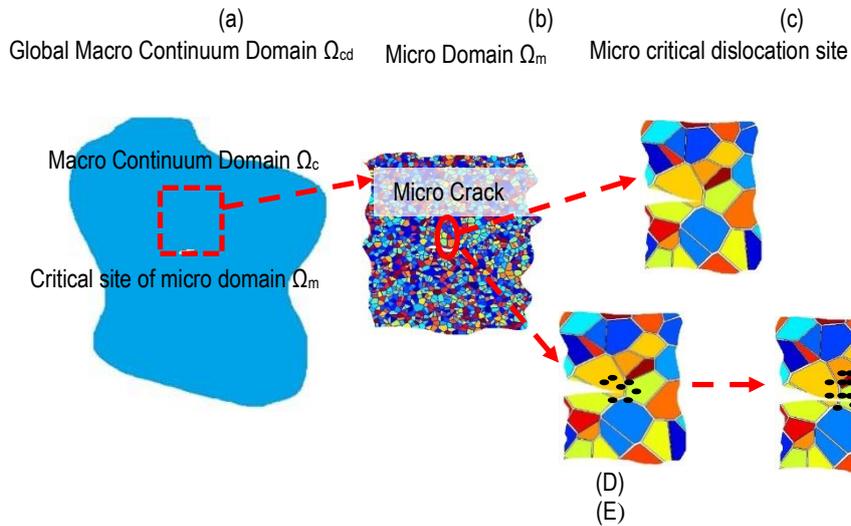


FIGURE:2 - (a) Macro Continuum domain with micro domain containing a microcrack (b) Schematic close-up view of micro domain, a region of heterogeneous intragranular and intergranular microstructural

polycrystalline material shows the pre-existing microcrack (c) Close view of critical intragranular and intergranular microstructural dislocation site containing microcrack tip in the absence of hydrogen. (d) Close view of critical intragranular and intergranular microstructural dislocation site containing microcrack tip in the presence of hydrogen accumulation near the crack tip (e) A critical amount of hydrogen concentration after a certain period of time due to stress assisted hydrogen diffusion at the micro cracks leads to catastrophic failure or premature brittle rupture.

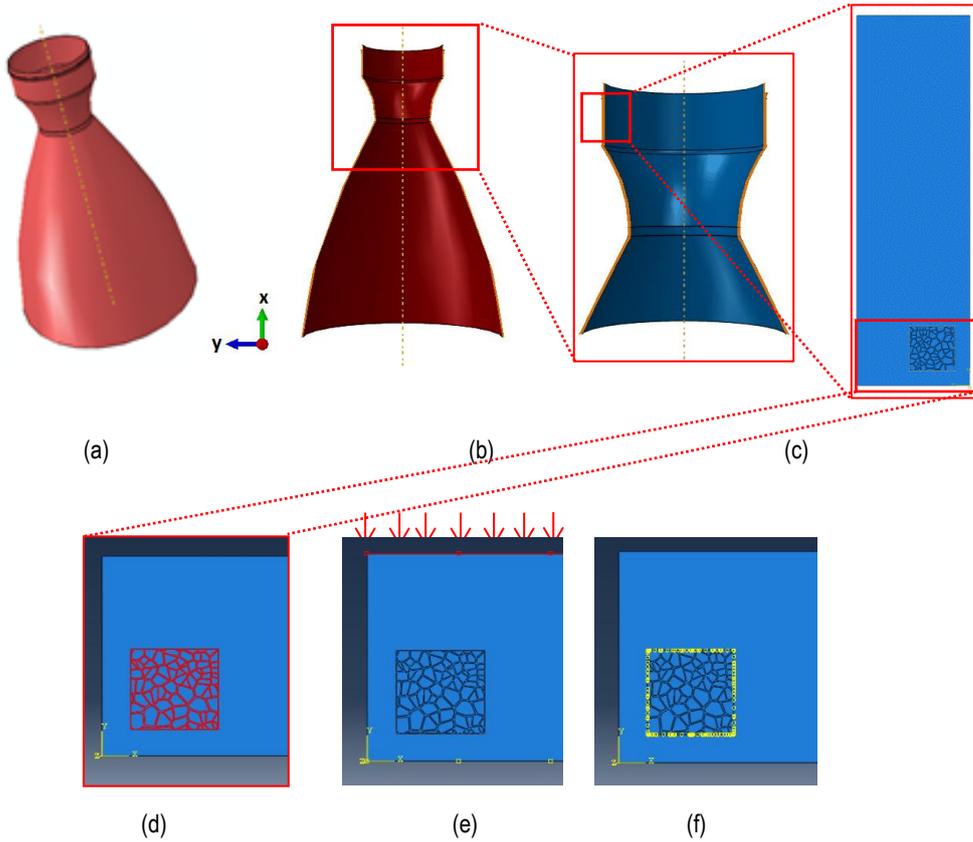


FIGURE: 3- (a) & (b) Space shuttle launcher thrust chamber geometry on the metre scale and a close-up view (c) Close-up view of the nickel layer of a thrust chamber cross section macro domain coupled with the micro domain (d) CMCD model without any cracks: Geometry with coupled continuum domain and micro domain and its close-up view. (Note: The area of the micro domain is $36 \mu\text{m}^2$. Average grain size in the micro domain is $1 \mu\text{m}$) (e) Boundary condition with hydrogen from environment entering into the material from outer surface to inner surface. (f) Tie boundary in yellow couples the micro and continuum domains.

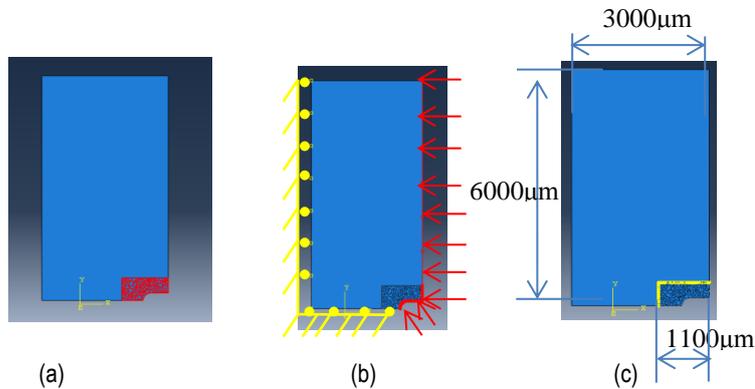
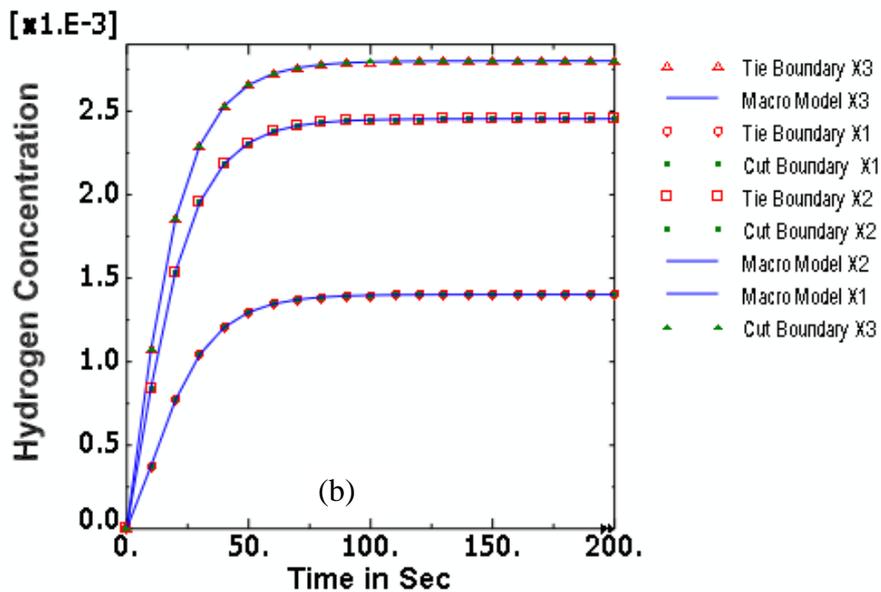
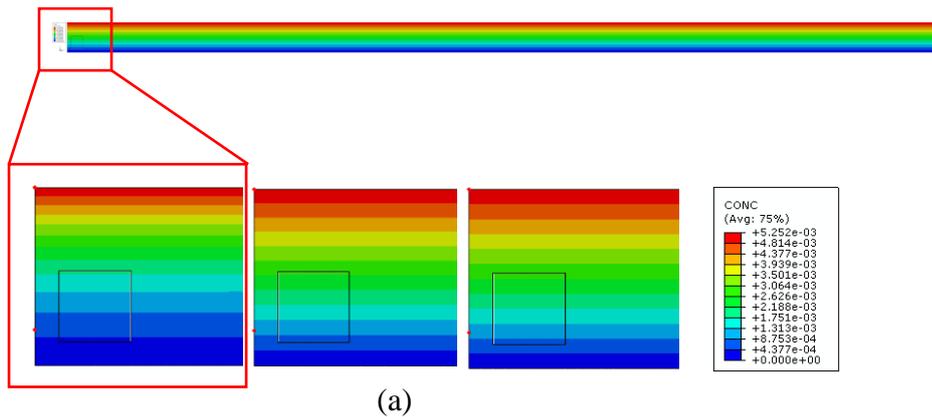
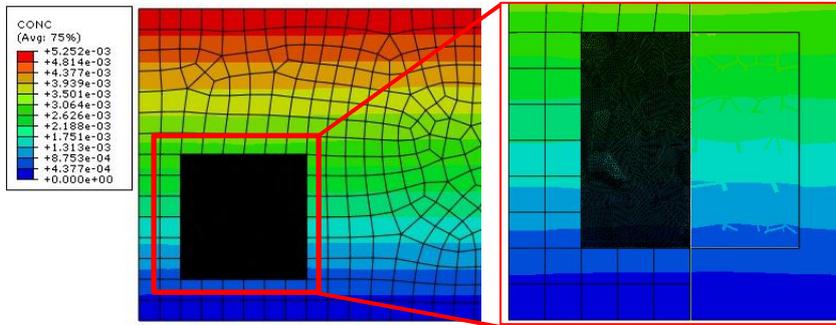
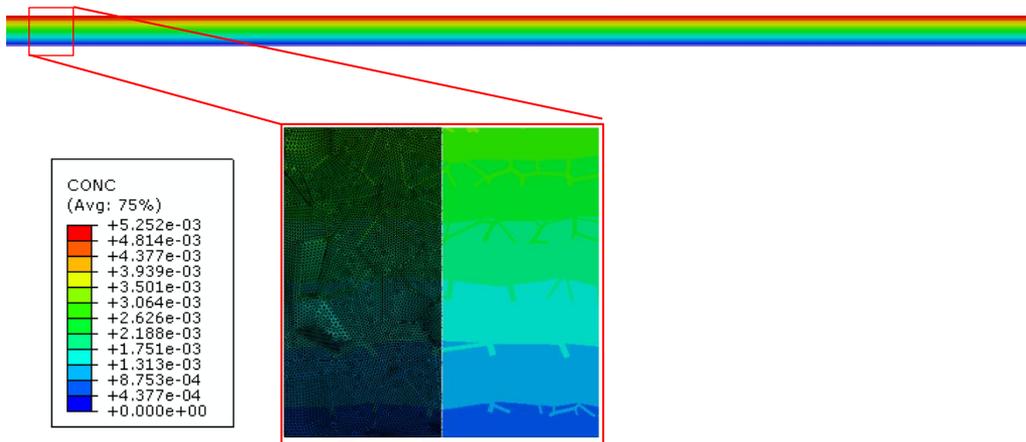


FIGURE: 4- Two dimensional axisymmetric CMCD Model with a crack in the form of sharp notch micro domain geometry is embedded with homogenized continuum domain near the critical site of sharp notch test piece. (Note: Notch radius $200\mu\text{m}$, crack length $=500\mu\text{m}$ and average grain size $=70\mu\text{m}$) (b) Coupling the micro domain with the continuum domain as tie boundary in yellow colour. (c) Boundary condition of the problem showing the hydrogen entry surface of the material from the environment.





(c) Results of tie boundary technique



(d) Results of cut boundary technique

FIGURE: 5- Contours of hydrogen concentration on a coupled two scale CMCD model without any crack. (a) Shows the hydrogen diffusion results of boundary technique at three different elapsed times of 20s, 60s and 400s respectively. Note: To validate the tie and cut boundary technique the CMCD model without crack has been analysed using the effective diffusion property in both macro and micro model. The diffusivity used in the model is $2 \times 10^{-12} \text{ m}^2/\text{s}$ (b) Plot shows the validation of the micro boundary technique model. The results shows the hydrogen diffusion concentration profile between macro model and micro model on tie boundary and

cut boundary technique at three different length from top to bottom names as X1,X2 and X3(i.e X1=7 μ m, X2=8 μ m and X3=11 μ m; (Note: same colour legend for all the figures). (c) & (d) Shows the hydrogen distribution in CMCD model based on a tie boundary technique and cut boundary technique respectively after an elapsed time of 400s. Homogeneous distribution of hydrogen in macro model and heterogeneous distribution of hydrogen in micro model are observed. On the sub-scale the diffusion through grain and grain boundary is resolved using substructure and submodel micro domain boundary method. The area of the micro domain is 36 μ m² and the average grain size of polycrystalline material in the micro domain is 1 μ m. Note: the diffusion properties used in intragranular region, intergranular region and macro domain are 9×10^{-14} m²/s, 4×10^{-10} m²/s and 2×10^{-12} m²/s respectively. The effective diffusion property used in macro domain for average grain size of 1 μ m is calculated based on a finite element microstructure homogenization method developed by authors and detailed descriptions of this technique can be found elsewhere [12].

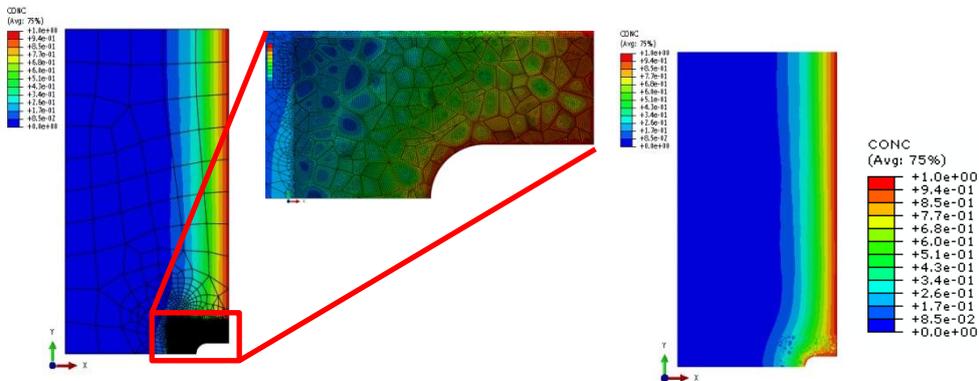
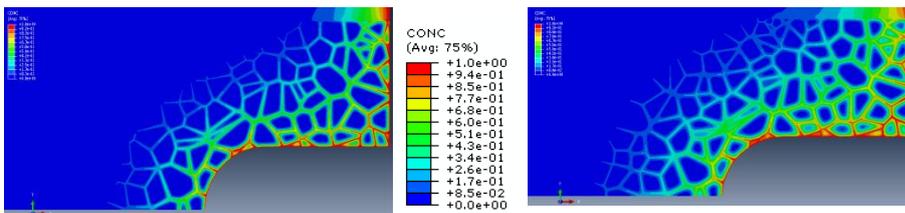


FIGURE: 6- Contours of hydrogen concentration on of a coupled two scale CMCD model with crack after 1×10^7 s. On the sub-scale the diffusion through intergranular and intergranular heterogeneous microstructure is resolved at two different time scale using substructure micro domain method. Macro-scale assumptions, homogeneous behaviour, are assumed at the larger scale. Note: the diffusion properties used in grain, grain boundary and macro domain are 9×10^{-14} m²/s, 4×10^{-10} m²/s and 1×10^{-13} m²/s.



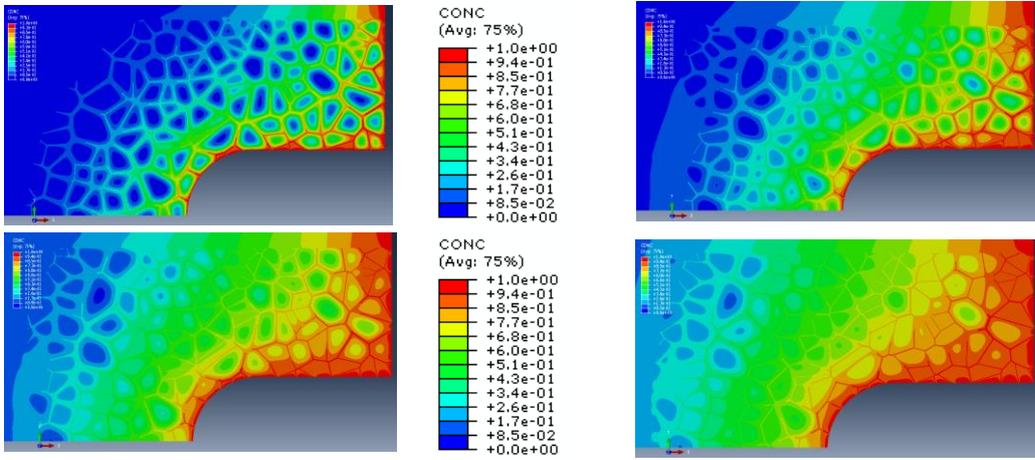


FIGURE: 7- Close view of the heterogeneous hydrogen diffusion and accumulation mechanism of the micro domain for various increasing times (elapsed times are as follows $t_1=2.29 \times 10^5$ s, $t_2=4.9 \times 10^5$ s, $t_3=1.13 \times 10^6$ s, $t_4=4.1 \times 10^6$ s, $t_5=6.1 \times 10^6$ s, $t_6=1 \times 10^7$ s) in the CMCD model with crack.