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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 behaviour 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 analyse 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.

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. [11,12,18–21]). 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

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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 modelled 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 modelled 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 using synthetic and real microstructures 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 modelled 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 Fig. 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

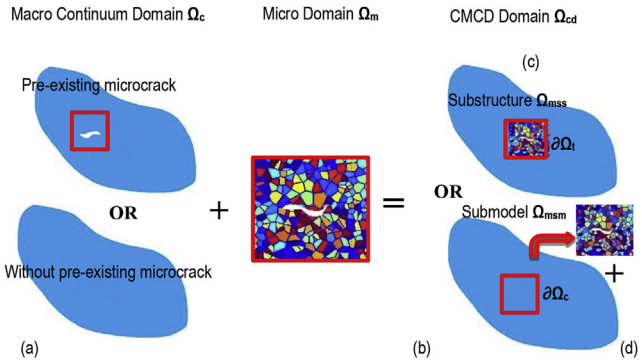

Fig. 1 – Schematic of the coupled microstructural and continuum critical dislocation site model using heterogeneous intragranular and intergranular microstructural domain as substructure or submodel.

solved as two decomposed problem as shown in Fig. 1(d). The detailed information about cut boundary and tie boundary methods can be found elsewhere [13,20]. 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,