Hierarchical Multiscale Analysis and Creep Cavitation Model-Based Creep Lifetime Prediction of New and Service-Exposed 9Cr-1Mo (Grade T91) Steel Boiler Tubes

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1. Introduction

Polycrystalline microstructure plays an important role in mechanical properties and creep behavior of steel alloys at elevated temperature, for example, boiler tubes in thermal power plants. Theory of crystal plasticity [1-2] forms the basis of grain-level (mesoscale) approaches to materials modeling using multi-scale strategies. The main feature of the theory of crystal plasticity is that it explicitly models discrete grains and slip systems, accounting naturally for the anisotropy of single crystal properties and texture evolution, main contributors to the anisotropic macroscopic response of crystalline solids. These theories provide a very predictive and robust theoretical framework to get a better understanding of polycrystal behavior that can lead to better continuum plasticity models. At elevated temperature, the inelastic behavior of metals will be rate-dependent, for which viscoplasticity should be considered. The viscoplasticity model can account for not only permanent plastic deformation but also creep deformation as a function of time. In this study, the crystal elasto-viscoplasticity (CEV) [3] will be implemented to describe the time-dependent isothermal, quasi-static, large deformation of Grade T91 ferritic/martensitic steel boiler tubes.

We present here a theoretical procedure for creep lifetime prediction of new and service-exposed Grade T91 alloy based on creep cavitation model and CEV. The value of stress concentration appears near triple junctions of hexagonal polycrystalline Grade T91 alloy will be evaluated and then implemented as the main driving force of creep failure in the creep cavitation model to predict creep lifetime of Grade T91 boiler tubes.

2. Multiscale Analysis Results

A computational experiment with molecular dynamics (MD) simulation will be carried out to estimate the anisotropic elastic moduli of single-crystalline body-centered cubic (BCC) Grade T91 ferritic steel alloy. In this study, Large-scale atomic/molecular massively parallel simulator (LAMMPS) is used to find out the three independent anisotropic elastic constants of Grade T91 alloy at 600°C. The obtained elastic constants are C11 = 164.82, C12 = 104.20 and C44 = 80.36 GPa, which will be used in the CEV-finite element analysis (CEV-FEA) of Grade T91 alloy.

Also in this study, the extended Taylor hypothesis [4-5] is implemented to consider the macroscopic response of individual crystal, which is related to macroscopic behavior of the polycrystal, this procedure is hereby called polycrystal homogenization. A quasi-2D model of hexagonal polycrystalline is then simulated in a commercial FEA software, ABAQUS, to find out the concentrated stress near triple junctions. High stress concentration is expected to occur along the boundaries of the three inner grains as depicted in Fig. 1 (colored grains). All the hexagonal grains are assigned with CEV behavior and the surrounding matrix obeys homogenized CEV response by averaging the mechanical behaviors of fifty grains with different crystal orientations. Ten random sets of crystal orientations are applied to the three inner grains to account for the effect of misorientation angle. As can be seen in Fig. 2, the effect of misorientation angle to the normal stress field along the boundaries of triple junction is distinct, and the stress concentration ratio reaches 1.5.

The value of concentrated stress can be implemented into the creep cavitation model [6], which takes into account the effect of thermodynamic barrier, number of critical nucleation and vacancy finding probability to estimate the lifetime of Grade T91 ferritic steel boiler tubes.

3. Conclusions

The CEV behavior of Grade T91 ferritic/martensitic steel boiler tubes has been thoroughly studied, formulated and simulated by using CEV-FEA and hierarchical multiscale analysis.

The stress concentration near triple junctions in polycrystalline Grade T91 alloy was analyzed, showing that the stress concentration highly depends on misorientation angles among grains, and the maximum ratio of concentrated stress to macroscopic stress could reach the value of 1.5.

With the stress concentration value, the creep lifetime of Grade T91 ferritic steel boiler tubes was estimated by using the creep cavitation model.

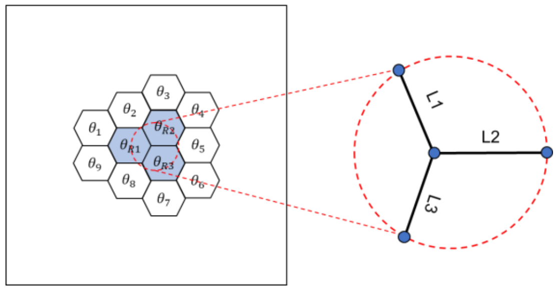

Fig.1 Geometry of the hexagonal polycrystalline model and notations of the grain boundaries

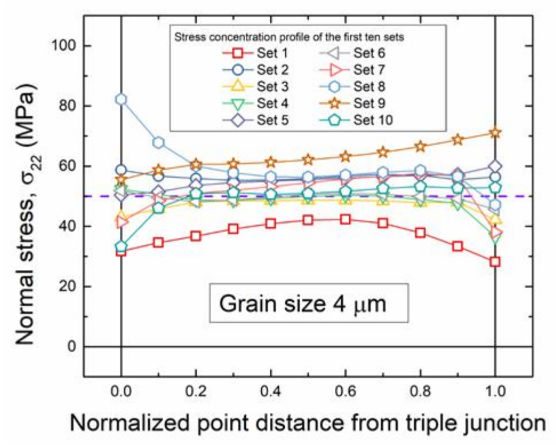

Fig.2 Normal stress profiles along the grain boundary L2 after 100,000 h of creep time computed using 10 sets of random crystal orientations

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