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Micromechanics based fatigue life prediction of a polycrystalline metal applying crystal plasticity

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ABSTRACT

The fatigue-life of a polycrystalline superalloy under symmetrical cyclic strain controlled loading at a temperature of 650 °C is investigated by numerical simulations on the micro-level, focusing on the inhomogeneous evolution of plastic deformation in a polycrystalline aggregate. A methodology (Zhang et al., 2011, 2013) to predict the low-cycle fatigue life by micro-level simulations along with statistical analysis is applied following the steps: (1) A statistically representative volume element (RVE) consisting of a number of crystal grains is constructed by Voronoi tessellation. Stresses and plastic strains are calculated by a crystal plasticity model including nonlinear kinematic hardening. (2) The RVE is subjected to repeated symmetric tensile-compressive loading. (3) The inhomogeneous stress and strain fields are statistically analyzed during the load cycles. (4) Failure by LCF is strain controlled and occurs if either of the quantities, standard deviation of longitudinal strain in tensile direction, maximum or statistical average of first principal strains in the RVE at the tension peak of cyclic loading reaches a respective critical value. (5) Using the present methodology, a family of failure curves for fatigue lives under different strain amplitudes can be predicted by varying the critical values. Finally, appropriate critical values can be identified by a respective cyclic experiment with only one strain amplitude.

1. Introduction

The investigations on metal low-cycle fatigue are usually related to metallurgical and mechanical aspects. Namely, the investigations often involve the micro-structure of the metal and its evolution, the response of stress and strain to different loading and the number of load cycles required to cause failure. Therefore, for low-cycle fatigue analysis, the descriptions on the mechanical behavior related to the microstructure of a metallic material under repeated loading are very important.

The metal fatigue mechanisms and mechanical behavior can be described at different scales and from different viewpoints, depending on which processes at which structural levels researchers choose to focus upon (cf. Manson, 1953; Coffin, 1954; Chaboche, 2008; Shenoy et al., 2008; McDowell and Dunne, 2010; Sangid et al., 2011; Zhang et al., 2013; Keshavarz and Ghosh, 2013; Huang et al., 2014; Sweeney et al., 2013; Sweeney et al., 2014a). Since the processes of fatigue failure in materials usually occur in a very small volume, a microstructural analysis is essential for experimental and computational investigations.

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Modern technological advances have made this possible, so that we can extend fatigue studies to very small scales or cross scale in order to clarify the role of material microstructure.

Polycrystalline metallic materials consist of a large number of crystal grains. At the grain level, its mechanical behavior is very inhomogeneous, since the grains are randomly orientated and the material properties of an individual grain are anisotropic with respect to elastic and plastic deformations due to its crystal lattice-array. To investigate the evolution of inhomogeneous deformation fields in a metallic material during low cycle fatigue, it is necessary to explore the micro-level plastic deformation and its accumulation, and the law of fatigue life with respect to the cyclic loading conditions. To achieve this objective, it is essential to select a reasonable scale for the analysis, a suitable constitutive model to reflect the cyclic plastic deformation mechanism at a relevant size level, and the corresponding fatigue model for service life analysis.

If the analysis is carried out at scales from 10^{-3} to mm by using a material representative volume element, representing the sizes from a crystal grain to a material test specimen, the results can be verified both qualitatively and quantitatively by using the conventional fatigue test machine and observation instrument (Zhang et al., 2013). For a polycrystalline metal, an appropriate representative element model should be able to describe the material's mechanical behavior at both the macroscale and the microscale. Such a material element contains a considerable number of grains, so that it can statistically reflect the typical material microstructural characteristics and the mechanical responses under realistic experimental conditions. On the other hand, it is adequately small to still represent a "material point" at the macroscale. This representative volume element (RVE) can be constructed by using a Voronoi polyhedron aggregation (Barbe et al., 2001; Kanit et al., 2003; Zhang et al., 2005). It should be emphasized that, different from classical RVE studies, the present RVE is used not only to reflect the homogenized properties but also to study the evolution of the inhomogeneous local deformation of a heterogeneous material (Ju and Chen, 1994; Ju and Tseng, 1996; Ju and Sun, 2001; Sun et al., 2003a,b; Zhang, 2004; Shenoy et al., 2008; Zhang et al., 2013).

The deformation of a crystalline grain in polycrystalline material can be split into the anisotropic elastic lattice distortion and the anisotropic crystal plastic slip caused by a large number of local stress-driven dislocations moving along the close-packed plane of atoms. These deformation mechanisms involving lattice distortion and crystal slip were discussed and investigated through establishing a crystal slip theory by Hill and Rice (1972), and Asaro and Rice (1977). Later, different algorithms under various configurations at finite deformations were suggested (cf. Peirce et al., 1983; Needleman et al., 1985; Kalidindi et al., 1992; Maniatty et al., 1992; Sarma and Zacharia, 1999), mainly to apply the crystal plasticity theory to numerical analysis of texture-forming. Further, improvements in computational schemes were made, in which the Cauchy stress was chosen as a basic variable and a mixed implicit and explicit algorithm matched to a user material subroutine of ABAQUS was established (Zhang, 2004; Zhang et al., 2005). In recent years, a Voronoi polyhedron aggregation has increasingly been employed for the analysis of three-dimensional microscopic inhomogeneous stress and strain fields of polycrystalline materials. The activation and development of different slip systems of each grain in the RVE, driven by the local stress, can be computed by taking account of the random grain orientations.

In order to understand the deformation evolution process in a heterogeneous metal at the micro-level under the low-cycle fatigue loading, suitable computations need to be performed to describe the material microstructural features, the microscale deformation mechanism and the variance of strains and stresses in a metal during the low-cycle loading process. To take into account the Bauschinger effect in a single crystal, which is important for fatigue analysis due to cyclic loading condition, Cailletaud (1992) introduced the back-stress and nonlinear kinematic hardening into the slip description at the level of each slip system. Subsequently, Hutchinson's power law (Hutchinson, 1976) was generalized by introducing the back stress into a crystal plasticity model (Feng et al., 2004), in which the Armstrong–Frederick type kinematic hardening rule (Armstrong and Frederick, 1966) was invoked to capture the Bauschinger effect. Moreover, for the purpose of accommodating the cyclic hardening feature of the slipping system, a modified evolution law for the back-stress with respect to the resolved shear stress on slip system was proposed by Zhang et al. (2011), by which the inhomogeneous deformation of a copper under cyclic loading and the subsequent yield of an aluminum after cyclic loading are studied by Zhang et al. (2013) and Hu et al. (2015), respectively.

The strains and stresses in a metallic material at the microscale are usually inhomogeneous due to the heterogeneity of the material's microstructure. At the micro-level, the inhomogeneity and heterogeneity for the microstructure and the deformation distribution will evolve with the loading cycles. As a result, a material changes gradually due to the evolution of residual deformations and stresses and the orientations and shapes of the grains. In order to characterize the evolution of material structure and behavior at various micro-scales, many investigations have been engaged (Abdeljaoued et al., 2009; Dunne et al., 2007; Guilhem et al., 2010; Taheri et al., 2011; Przybyla and McDowell, 2010; Dingreville et al., 2010; Sweeney et al., 2013; Sweeney et al., 2014b; Zhang et al., 2011). In the process of a material deformation under cyclic loading, the evolutions of the material inhomogeneity may continue until the fatigue failure occurs, which can be described by statistical distribution with two characteristic parameters; i.e., the mean value and standard deviation (Zhang et al., 2013).

A primary objective to investigate fatigue is to establish a rational methodology for fatigue life prediction. Here, the fatigue life means the cycle number to failure of a material specimen under cyclic loading with a macro uniform deformation. The Manson–Coffin equation (Manson, 1953; Coffin, 1954) or its modification was widely used