International Journal of Plasticity 54 (2014) 229–246

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

A study of fatigue crack tip characteristics using discrete dislocation dynamics

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ARTICLE INFO

Article history:
Received 15 February 2012
Received in final revised form 26 August 2013
Available online 8 September 2013

Keywords:
Crack tip
Cyclic response
Discrete dislocation dynamics
Disclocation climb
Grain boundary

ABSTRACT

The near-tip deformation of a transgrannular crack under cyclic loading conditions has been modelled using discrete dislocation dynamics (DDD) with both dislocation climb and dislocation-grain boundary (GB) penetration considered. A representative cell was built to model the constitutive behaviour of the material, from which the DDD model parameters were fitted against the experimental data. The near-tip constitutive behaviour was simulated for a transgranular crack in a polycrystalline nickel-based superalloy. A phenomenon of cyclic creep or strain ratchetting was reproduced, similar to that obtained using viscoplastic and crystal-plastic models in continuum mechanics. Ratchetting has been found to be associated with dislocation accumulation, dislocation climb and dislocation-GB penetration, among which dislocation climb seems to be the dominant mechanism for the cases considered at elevated temperature. Ratchetting behaviour seems to have a distinctive discrete characteristic in that more pronounced ratchetting occurred within slip bands than elsewhere. Multiple slip systems were activated in grains surrounding the crack tip, as opposed to single active slip system in grains away from the crack tip. The present DDD results show that, the near-tip ratchetting strain ahead of the crack tip seems to be a physical phenomenon, which may be of particular significance for developing a physical-based model of crack growth.

1. Introduction

Mechanical response and lifetime assessment of engineering materials under cyclic loading conditions has been a continuing driver for the development of new/improved constitutive material models, notably but not exclusively of those reported recently (Chaboche, 2008; Taleb and Cailletaud, 2011; Xiao et al., 2012; Yu et al., 2012; Pham et al., 2013; Chaboche et al., 2013), where aspects of cyclic response, such as cyclic hardening/softening and saturation (Pham et al., 2013), dynamic strain ageing (Yu et al., 2012; Chaboche et al., 2013) and strain ratchetting (Abdel-Karim, 2010; Taleb and Cailletaud, 2011), have been carefully studied. Although these studies have significantly enhanced our understanding of the overall stress–strain behaviour of engineering materials under cyclic loading conditions, the immediate impact of such a progress is often on the studies of fatigue crack initiation. Fatigue crack propagation, on the other hand, despite of being extremely important to damage tolerance design implemented virtually on all fracture critical components and structures, has not always benefited immediately from the most recent developments.

Mechanistic understanding of fatigue crack growth may be traced back to Rice (1967) who provided a seminal analysis of stress and strain fields near an idealised stationary crack tip under tensile and anti-plane shear cyclic loadings. It was found

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0749-6419/$ - see front matter
http://dx.doi.org/10.1016/j.ijplas.2013.08.016

that the crack-tip cyclic plastic deformation may be adequately determined by the variation in a stress intensity factor, and the reversed plastic-zone size due to load reversal is one quarter of the size of the maximum plastic zone. Considerable analytical research has since been carried out to study the controlling parameters of crack-tip deformation and crack propagation, notably including the well-known Hutchinson–Rice–Rosengren (HRR) field for power-law hardening materials; the RR (Riedel and Rice, 1980) and the HR (Hui and Riedel, 1981) fields for power-law creep materials. Numerous finite element (FE) analyses have been carried out to model the crack-tip deformation using cyclic plasticity and crystal plasticity constitutive models (e.g., Sehitoglu and Sun, 1991; Pommier and Bompard, 2000; Zhao et al., 2001; Tvergaard, 2004; Zhao and Tong, 2008). Keck et al. (1985) demonstrated the dependency of crack-tip stress–strain field and plastic-zone size on loading frequency and hold time, where low frequency and introduced hold time at maximum load led to increased crack-tip deformation and plastic-zone size. Characteristic strain ratchetting near a crack tip was found by Zhao et al. (2001) and Zhao and Tong (2008), where tensile strain normal to the crack plane was found to accumulate progressively. Flouriot et al. (2003) investigated the crack-tip strain field in a single crystal using the elasto(visco)-plastic model developed by Meric et al. (1991). Their results also showed strain ratchetting occurring primarily in some of the localised slip bands. Using the same material model (Meric et al., 1991), Marchal et al. (2006) found that ratchetting appears to be on octahedral slip systems and the amount of ratchetting depends on the distance from the crack tip. Dunne et al. (2007) used a simplified crystal plasticity model to study the low cycle fatigue crack nucleation. Their predicted locations of the persistent slip bands coincided well with the experimentally observed sites of crack nucleation. Using a crystal plasticity model (Busso et al., 2000), Lin et al. (2011) studied the near-tip deformation of a transgranular crack in a compact tension specimen for a polycrystalline nickel alloy. Ratchetting phenomenon was once again found near the crack tip, and the shear deformation on the slip planes was found to accumulate with the increase of the number of cycles.

Nickel-based superalloys have been used for gas turbine discs applications, where fatigue and creep deformation is of primary concerns. Extensively studies (for example, Meric et al., 1991; Nouailhas and Cailletaud, 1995; Dalby and Tong, 2005; Zhan and Tong, 2007a, b; Lin et al. 2011; Tong et al., 2011) have been carried out to understand the material constitutive and crack growth behaviour at elevated temperature. It is well known that the interaction between dislocations and material microstructure, e.g., grain boundary (GB) and the second phase γ' precipitate, plays an important role in dictating the stress–strain response of the material. Modelling of dislocation-microstructure interaction has been attempted by formulating the constitutive laws. For instance, Fedelich (1999, 2002) introduced some microstructure parameters, including precipitate size, channel width and lattice mismatch, into his dislocation-based crystal plasticity constitutive law, and investigated the influence of microstructure parameters on the mechanical behaviour of a single crystal Ni-based superalloy. Busso et al. (2000) proposed a gradient- and rate-dependent crystallographic formulation for a single crystal Ni-based superalloy CMSX4, and investigated the effects of precipitate size and channel width on mechanical behaviour. Shenoy et al. (2008) formulated a rate-dependent, microstructure-sensitive crystal plasticity model for a polycrystalline Ni-base superalloy, which has the capability to capture first-order effects on the stress–strain response due to grain size, precipitate size distribution and precipitate volume fraction. Tinga et al. (2010) introduced the interaction of dislocations with the microstructure (such as the dislocations shear and climb over the precipitates) into a single crystal dislocation density-based constitutive model to capture the non-Schmid response of a nickel alloy. Vattré and Fedelich (2011) developed a micromechanical dislocation density-based constitutive model with a pseudo-cubic slip law which improved the estimation of the strain hardening anisotropy. Although both the material microstructure and dislocation density evolution were incorporated, these constitutive models were formulated only within a continuum plasticity framework. Since dislocation density-based constitutive continuum models can consider the interaction between dislocations and internal material microstructures, such as grain boundaries, secondary phases and dislocation cells, many researchers have recently focused their efforts on these approaches, leading to significant developments in this area (notably, Fan and Yang, 2011; Hamelin et al., 2011; Barlat et al., 2013; Bertin et al., 2013; Franz et al., 2013; Hansen et al.,2013; Li et al., 2013; Resende et al., 2013; Shanthraj and Zikry, 2013). However, as pointed out by Berdichevsky and Dimiduk (2005), the application of continuum plasticity is questionable at the scale of the dislocation structure. This issue becomes particularly crucial for typical microstructures of nickel alloys, since the use of dislocation density $\rho(x)$ as an independent local variable in the mesoscopic constitutive models cannot be justified by a spatial averaging at the scale of channel width (Vattré and Fedelich, 2011). When a crack is concerned, dislocations tend to be organised into heterogeneous dislocation structures (such as slip bands) within an area of micron or sub-micron size ahead of the crack tip. Since continuum constitutive models only consider dislocation evolution phenomenally or statistically, they cannot accurately describe these local heterogeneous dislocation structures and capture the local non-homogeneous deformation field ahead of a crack tip.

To consider the discreteness of dislocation structure ahead of a crack tip, Cleveringa et al. (2000) carried out a two dimensional (2D) discrete dislocation dynamics (DDD) analysis of crack-tip deformation field and crack growth in a FCC (face-centre-cubic) single crystal under mode I loading. It was found that the local stress concentration associated with discrete dislocation patterning ahead of the crack tip can lead to stress levels much higher than the yield stress, and indeed high enough to cause atomic separation. Van der Giessen et al. (2001) performed a 2D DDD simulation of the crack-tip deformation field for a stationary plane strain mode I crack. Their results showed that crack-tip deformation field and dislocation structure depend on slip system orientation; and the opening stress in the immediate vicinity of the crack tip is much larger than that predicted by continuum slip theory. Deshpande et al. (2003) modelled edge-cracked single crystal specimens of varying sizes subject to both monotonic and cyclic loading using 2D DDD simulation. It was found that the fatigue crack growth threshold decreases substantially with the crack size when it is below a critical value. Brinckmann and Van der Giessen