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Fatigue crack nucleation: Mechanistic modelling across the length scales

F.P.E. Dunne

Department of Materials, Imperial College, London SW7 2AZ, UK

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ABSTRACT

This paper presents an assessment of recent literature on the mechanistic understanding of fatigue crack nucleation and the associated modelling techniques employed. In particular, the important roles of (a) slip localisation and persistent slip band formation, (b) grain boundaries, slip transfer and interfaces, (c) microtexture and twins, and (d) nucleation criteria and microcracks are addressed in the context of the three key modelling techniques of crystal plasticity (CP), discrete dislocation (DD) plasticity and molecular dynamics (MD) where appropriate. In addition, the need for computational fatigue crack nucleation methodologies which incorporate mechanistic understanding is addressed.

Key challenges identified include (i) the overall need for multiscale models for fatigue crack nucleation which are continuum-based but mechanistically informed; (ii) full (3D) crystal slip models to capture slip localisation at a DD level; (iii) MD modelling methodologies for slip transfer to inform DD models; and (iv) rigorously validated dislocation structure models at the DD and CP levels.

1. Introduction

This paper aims to assess representative current research in mechanistic understanding and modelling in fatigue crack nucleation through to the development of predictive capability in engineering practice. It is by no means exhaustive, and hence because of space limitations, apologies are due to those authors not explicitly cited. In order to introduce the scope of work addressed, the paper begins with a recapitulation of an early crack nucleation model, together with a brief overview of the importance of microstructure in fatigue. The key modelling techniques across the microstructural length scales are then introduced and are followed by the assessment of mechanistic understanding and modelling of fatigue crack nucleation. In this paper, the term fatigue crack nucleation is used to refer to the deformation and failure processes which occur under cyclic loading at the key controlling microstructural features and at the length scale appropriate to those features. Often, this is the scale relevant to grains, twins and boundaries, slip localisation and persistent slip band formation.

The first rigorous mechanics-based fatigue crack nucleation criterion proposed is likely that developed by Stroh [1] in 1954. In this model, shown schematically in Fig. 1, a line of discrete dislocations, forming a persistent slip band (PSB), is contained within an infinite elastic medium and inclined at a given angle to a remote nominal stress σ_0. The resulting normal stresses σ_n at the termination of the PSB are developed in terms of the length of the PSB, l, its orientation, θ, and the distance from its end, r, as follows

$$\frac{\sigma_n}{\sigma_0} = \frac{3}{2}\left(\frac{l}{r}\right)^{1/2} \sin\theta \cos\frac{1}{2}\theta \tag{1}$$

Stroh went on to introduce a fracture criterion based on the material's toughness, and the dislocation density (or number of dislocations within the PSB length l). He therefore recognised the link between PSB formation and crack nucleation, and also the importance of local dislocation density. While the form of model proposed by Stroh has found quite widespread importance in facet fatigue nucleation in titanium alloys, its direct application to fatigue crack nucleation problems in general has been less explicit, for a whole range of reasons to be addressed shortly, but in summary, because the appropriate microstructural-level information needed was not available. However, many current approaches to modelling fatigue crack nucleation are in fact closely related to the Stroh model.

In order to introduce the microstructural detail and its importance in fatigue crack nucleation, let us examine briefly three examples which include single crystal copper, 316 stainless steel and a commercial titanium alloy. Ahmed et al. [2] investigated the development of dislocation structures and PSBs in single crystal copper, orientated for single slip, subject to tension–compression, using electron channelling contrast imaging (ECCI) within a scanning electron microscope. Fatigue cracks nucleated and grew along some but not all of the PSBs and an example is shown in

E-mail address: fionn.dunne@imperial.ac.uk

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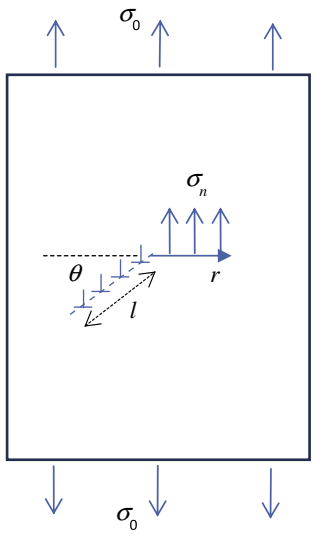

Fig. 1. Schematic diagram of the Stroh crack nucleation model showing a PSB of length *l*, orientated to a remote stress and in an infinite elastic medium.

Fig. 2a. More recently, Pham et al. [3,4] have examined the development of PSBs and dislocation structures in 316 steel using TEM, an example of which is shown in Fig. 2b, forming within individual grains but contained in the bulk of the polycrystal. A relationship exists between the ladder-free PSBs and fatigue cracking, but is not straightforward [4]. In the third example, micromechanical fatigue testing on a titanium alloy is investigated in which the role of particular microstructural features (including the alpha and beta phases) is assessed [5] and Fig. 2c identifies an alpha grain well-orientated for prismatic slip and the resulting highly localised, heterogeneous slip developed.

The progressive complexity, from single to polycrystal structures with differing crystal lattices, in the highly heterogeneous nature of the development of slip, and its dependence on microstructural features of differing length scale, are immediately clear from these examples. It thus becomes apparent why it is that rigorous models such as that of Stroh [1] for fatigue crack nucleation have not yet been completely successful. What is clear also is that any predictive technique must be based on full knowledge of the key microstructural features which may exist and remain important over a range of differing length scales even within a single material system. It is argued from the start that one of the key challenges in fatigue modelling is in identifying the appropriate, key controlling length scales and microstructural features for a given material system.

In passing, it is noted that there already exist some excellent relevant reviews of fatigue research including those of Chan [6], McDowell and Dunne [7], Mughrabi [8] and Sangid [9]. The present paper aims to assess current knowledge of the key length scales and microstructural features from which successful mechanistically-informed modelling strategies might be developed. The paper is structured such that firstly, a brief overview of commonly used generic modelling techniques (namely, molecular dynamics, discrete dislocation and crystal plasticity) is presented, and this is then followed by a presentation of a small but relevant subset of the research literature appropriate to fatigue crack nucleation which addresses (a) slip localisation and PSBs, (b) grain boundaries,

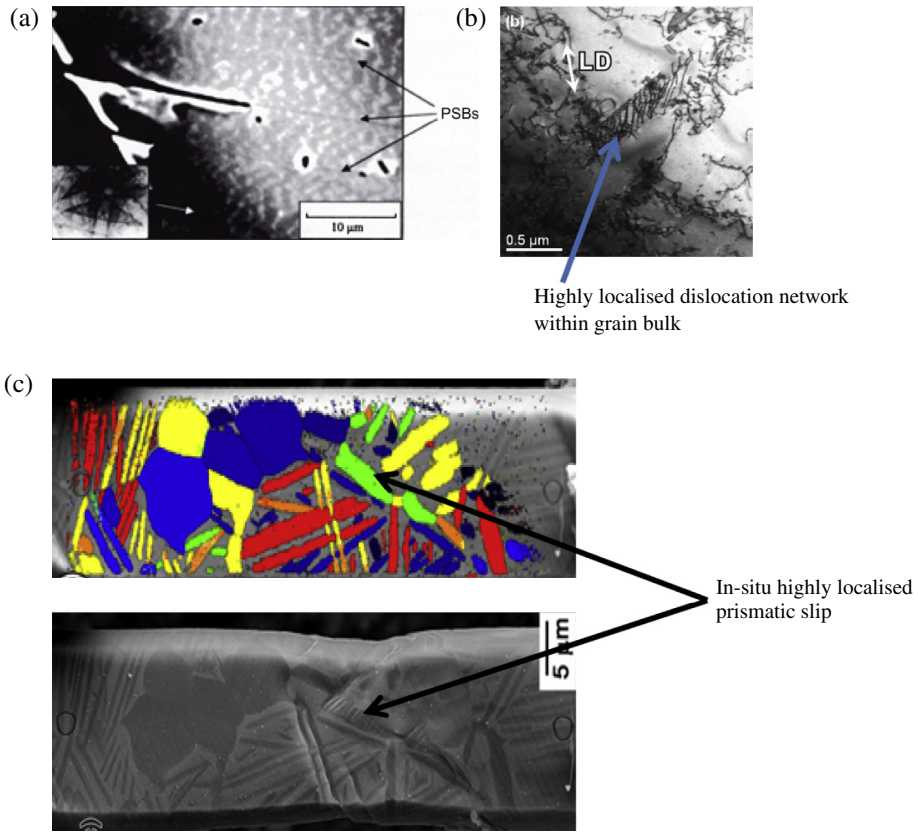

Fig. 2. (a) PSB and fatigue crack nucleation within single-crystal copper [2]; (b) dislocation structure within a grain in polycrystalline 316 steel [3] and (c) localised prismatic slip in a titanium alloy [5].