International Journal of Fatigue 116 (2018) 90–105

Contents lists available at ScienceDirect

International Journal of Fatigue

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

A grain-scale model for high-cycle fatigue degradation in polycrystalline materials

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ARTICLE INFO

Keywords:
High-cycle fatigue
Polycrystalline materials
Micro-mechanics
Intergranular degradation
Boundary element method

ABSTRACT

A grain-scale three-dimensional model for the analysis of fatigue intergranular degradation in polycrystalline materials is presented. The material microstructure is explicitly represented through Voronoi tessellations, of either convex or non-convex domains, and the mechanics of individual grains is modelled using a boundary integral formulation. The intergranular interfaces degrade under the action of cyclic loads and their behaviour is represented employing a cohesive zone model embodying a local irreversible damage parameter that evolves according to high-cycle continuum damage laws. The model is based on the use of a damage decomposition into static and cyclic contributions, an envelope load representation and a cycle jump strategy. The consistence between the cyclic damage and the action of the external loads, which contribute to the damage due to the redistribution of intergranular tractions between subsequent cycle jumps, is assessed at each solution step, so to capture the onset of macro-failure when the external actions cannot be equilibrated anymore by the critically damaged interfaces. Several numerical tests are reported to illustrate the potential of the developed method, which may find application in multiscale modelling of fatigue material degradation as well as in the design of micro-electro-mechanical devices (MEMS).

1. Introduction

Materials fatigue degradation is a common cause of structural failure in several applications in the automotive, aerospace, maritime and oil industries [1–5]. The design of engineering components subjected to cyclic loads has been traditionally based on phenomenological semi-empirical tools, such as the Whöler σ-N curves [6], Basquin's power laws [7] or Goodman-type diagrams [8]. More recently, the analysis of fatigue induced cracks initiation and propagation has been addressed employing continuum damage mechanics [9] or fracture mechanics [10,11,4] approaches, within the framework of safe-life, fail-safe or damage-tolerance design methodologies.

The above tools have been and are currently used in the analysis and design of macroscopic mechanical components subjected to cyclic loads. However, the last few decades have seen a surge of interest in the study and modelling of materials at the micro/nano scales [12–14]. Remarkable interest has been attracted by investigations at the *meso-scale*, with the explicit representation of the heterogeneous constituents of materials often assumed as homogeneous at the macro-scale; outstanding examples are provided either by the micro-mechanical studies on fibre-reinforced composites [15–17], with the explicit representation of individual laminae or even fibres, matrix and related interfaces, or by the analysis of polycrystalline aggregates, with the direct account of individual grains and intergranular interfaces [18,13].

The trend towards computational micro-mechanics has different motivations. From a *macroscopic* point of view, it is driven by the scientific interest for better understanding of materials behaviour, beyond their phenomenological representation, and the consequential technological drive towards the improvement of materials performances by chemical pathways, as for example in the case of grain-boundary engineering [19], or by topological/morphological control of the microstructure, as in the manufacturing of foam and lattice materials [20,21]. From an inherently *microscopic* point of view, such interest is often related to the rapid development and widespread use of micro-electro-mechanical systems (MEMS), today routinely employed and well established in several engineering applications as transducers, gears and mechanical linkages [22]. In any case, the rapid development of computational micro-mechanics has certainly benefitted from the development of experimental techniques for materials characterisation [23,24] and from the current affordability of high performance computing (HPC) [25].

In the sketched background, the study of materials damage and failure micro-mechanisms has assumed particular importance, as it allows the enhanced understanding of damage nucleation across length

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https://doi.org/10.1016/j.ijfatigue.2018.06.010
Received 27 January 2018; Received in revised form 5 June 2018; Accepted 7 June 2018
Available online 15 June 2018
0142-1123/

scales in engineering applications [26] and it may find direct application in the design of MEMS [27–30]. In this study, we focus on modelling of degradation and failure in polycrystalline aggregates subjected to cyclic loads. Polycrystalline materials, either metals or ceramics, are widely employed in a diverse range of engineering applications. Polycrystalline silicon, or polysilicon, is routinely used for the production of MEMS components, which are often subjected to cyclic loads [31–33].

The microstructure of polycrystalline materials is characterised by the shape and crystallographic orientation of the grains and by the physical and chemical properties of the intergranular interfaces, which play an important role in their micro-mechanics. Several computational techniques have been developed for the analysis of polycrystalline materials at the micro-scale and for the study of their mechanical, damage and failure behaviour [34,35]. In particular, grain-scale models have been developed for material homogenisation [36,37], quasi-static failure [38,39] and stress corrosion cracking [40–43]. Also the progressive fatigue degradation of polycrystalline aggregates subjected to cyclic loads has been addressed in the literature. Manonukul and Dunne [44] and Cheong et al. [45] have developed crystal plasticity finite element frameworks with fatigue crack initiation criteria based on the accumulation of slip to quantify fatigue damage and crack initiation in low and/or high-cycle fatigue of polycrystalline aggregates. A review of the grain-scale, or microstructure-sensitive, computational models for fatigue in polycrystalline or poly-phase materials can be found e.g. in Refs. [13,46]. Several of such studies are often devoted to microstructures in which the accumulation of plastic slip is the dominant mechanism triggering the initiation of fatigue cracks at the grain scale. On the other hand, Jalalahmadi et al. [28] have developed a Voronoi finite element model (VFEM) for the analysis of fatigue damage and failure in MEMS; they employed a stress reversal based quasi-brittle damage evolution law suitable for fine-grain metal microstructures with highly confined plasticity, to model intergranular crack initiation and propagation stages and used it to investigate the effects of microstructure randomness on the fatigue of MEMS. The approach was extended to three-dimensional aggregates by Bomidi et al. [47].

In this work, a three-dimensional (3D) grain-scale boundary integral formulation for the analysis of polycrystalline aggregates under cyclic loading is proposed. Only intergranular fatigue degradation is considered here: the formulation is then suitable for aggregates/conditions in which plastic slip is absent or highly confined and then negligible [48–50]. Such conditions are often met in fine-grain MEMS applications [47]. The method is based on a grain-boundary integral approach previously developed and applied for computational material homogenisation [51,52], quasi-static intergranular and transgranular degradation and failure [53–59], hydrogen assisted stress corrosion cracking [60] and multiscale analysis of damage initiation, evolution, coalescence and fracture of polycrystalline components [61,62]. The formulation is based on a boundary integral representation of the mechanics of the individual grains, coupled with a cohesive zone model of the progressive degradation of the intergranular interfaces. In this work, to model fatigue degradation, the intergranular damage is decomposed into a contribution induced by the cyclic loads and a contribution from the quasi-static action of the applied loads, as it is often done in high-cycle fatigue analysis. This *damage decomposition* is used in conjunction with an *envelope load representation* of the external cyclic actions and a *cycle jump strategy* that, due to the practical unfeasibility of cycle-by-cycle analysis of high-cycle problems, is adopted to render the computation amenable. The formulation offers the advantage of expressing the micro-mechanical problem in terms of intergranular displacements and tractions only, which are then directly used in the expression of the traction-separation laws. Moreover, since only the discretisation of the grain boundaries is required, the methodology offers a simplification of the data preparation stage and a reduction of the number of degrees of freedom required by the micro-mechanical analysis, with resulting computational benefits.

The paper is organised as follows. The details about the generation of the analysed artificial polycrystalline morphologies are given in Section 2, where also a strategy for the generation of non-convex aggregates is described. The grain-boundary formulation is described in Section 3, where the employed boundary integral equations, the interface laws embodying fatigue degradation laws and the system solution are addressed. In particular, the description of the strategy used to model the intergranular degradation is described in Section 3.3, where the damage evolution decomposition is described and discussed on the background of the approaches used in the literature to address fatigue degradation; the envelope load approach and the cycle jump strategy are discussed in Section 3.4. Section 4 reports on the numerical tests performed using the developed method. Some discussion about the obtained results and an outline of possible further developments is given in Section 5, before the *Conclusions*.

2. Generation and meshing of artificial crystal aggregates

The first essential item of the proposed framework is a suitable artificial representation of polycrystalline microstructures. In this study, the fatigue behaviour of crystal aggregates contained within the volume $\mathscr{V}$, bounded by the surface $\mathscr{B} = \partial\mathscr{V}$, is considered. The polycrystalline aggregates are modelled employing a multi-region boundary element formulation [63], in which each different region represents an individual grain, with its own specific crystallographic properties and orientation in space.

Several different techniques have been used in the literature to represent polycrystalline aggregates, with resulting representations varying from the most schematic, see e.g. Ref. [64], to the most realistic, see e.g. Ref. [65] where the microstructure representation is based on 3D X-ray diffraction contrast tomography. In this work, the analysed morphologies are generated through Voronoi [37,66] or more general Laguerre [67–69] tessellations of the analysed domain $\mathscr{V}$. Such algorithms are relatively simple, yet mathematically well defined, space filling geometric subdivisions of the considered volume that provide suitable first-order approximations of real polycrystalline microstructures. Each Voronoi/Laguerre cell, which an individual grain g, is a convex polyhedron with the boundary S^g comprised of the union of *flat* convex polygonal faces F_n^g with $n = 1, ..., N_f^g$ and N_f^g denoting the number of faces of g. The tessellations can be practically built using open source software packages such as `Voro++` (http://math.lbl.gov/voro++/) [70] or `Neper` (http://neper.sourceforge.net) [66]. In this study, `Neper` has been employed; however, what follows can be applied also if other software packages are adopted for generating the domain tessellations.

In several studies, generally concerned with material homogenisation, the considered polycrystalline domains $\mathscr{V}$ have typically cubic or prismatic shape and contain a certain number of grains that are subsequently analysed with the aim of identifying some representative volume elements (RVEs), see Fig. 1. Cubic or prismatic boxes, and in general convex domains, can be straightforwardly generated with available software packages, which often provide methods for cutting grains or aggregates. However, the cutting operation, by its own nature, is not generally suitable for the generation of non-convex domain. With the aim of considering either convex or non-convex polycrystalline components, we have developed a dedicated technique for the tessellation of non-convex domains, similar to that used in Ref. [47]. The method is described next.

The non-convex domain $\mathscr{V}$, bounded by the surface $\mathscr{B} = \partial\mathscr{V}$, is considered; $\mathscr{V}$ can be enclosed within the parallelepiped bounding box $\mathscr{C}$. The tessellation of $\mathscr{V}$ is articulated in the following different stages, as illustrated in Fig. 2. (a) *Seeds generation*: initially, a certain number of seeds, with their associated weights if Laguerre tessellations are employed, is scattered within the box $\mathscr{C}$, so to achieve the target grains density. In the generation, for reducing the number of small geometrical entities, namely short edges and small faces, which would induce subsequent excessive mesh refinements, an additional hardcore