Computers and Structures xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Computers and Structures

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

On the effect of grains interface parameters on the macroscopic properties of polycrystalline materials

Ahmad Akbari [a,b,*], Pierre Kerfriden [b], Stéphane Bordas [c,d,*]

[a] Department of Mechanical Engineering, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran
[b] Cardiff University, School of Engineering, Cardiff CF24 3AA, Wales, UK
[c] Visiting Professor, Institute of Research and Development, Duy Tan University, K7/25 Quang Trung, Danang, Vietnam
[d] University of Luxembourg, Department of Computational Engineering Sciences, Faculty of Science, Engineering and Communication, University of Luxembourg, 6 Avenue de la Fonte, 4364 Esch-sur-Alzette, Luxembourg

ARTICLE INFO

Article history:
Received 8 May 2017
Accepted 14 September 2017
Available online xxxx

Keywords:
Polycrystalline microstructure
Cohesive interface
Multiscale modelling
Computational homogenisation
Yield surface
Stress-strain curve

ABSTRACT

In this paper, the influence of microscopic parameters on the macroscopic behaviour of polycrystalline materials under different loading configuration is investigated. Linear elastic grains with zero-thickness cohesive interfaces are considered at the microscale with in depth introduction of effective parameters. A multiscale method based on homogenisation technique is employed to bridge the scales. In order to minimize the homogenisation error, a representative volume element (RVE) of the microscopic structure is statistically determined to be used in the numerical analysis. For each loading condition of the RVE, several numerical examinations are conducted to illustrate the relationship between the microscopic parameters. Finally, the effects of microscopic critical fracture energies, maximum tensile and shear strengths of grain interfaces on the mechanical properties, i.e. stress-strain curve and yield surface at the macroscale are discussed in details. It is shown that macroscopic yield surface and stress-strain curves can be used to characterise the microscopic properties.

1. Introduction

Brittle failure in polycrystalline materials is usually due to inter-granular fracture: Cracks can grow along the interface between the grains. In trans-granular fracture, cracks propagate into the grains and the structure displays a more ductile response due to the plastic behaviour of the grains. The brittleness of inter-granular fracture is caused by the elastic behaviour of bulk grains which release more energy than the amount of energy needed for dissipation at the inter-granular cracks. The more energy released from the elastic grains, the faster the cracks propagate and the more brittle response is expected. A significant research on the failure of polycrystalline materials has been done, e.g. experimental studies can be found in Anil et al. [5], Bellante et al. [6], Luo et al. [21], Carolan et al. [9], and analytical/computational modelling can be found in Sakai et al. [32], Zavattieri and Espinosa [45], Sukumar et al. [37], Rollett et al. [31], Sfantos and Aliabadi [34], Verhoosel and Gutiérrez [41], and Paggi and Wriggers [30]. Researchers observed that inter-granular cracks are the main cause of crack initiation and propagation at the microscale which leads to the brittle failure of the structure from a macroscopic point of view [25,43]. In computational modelling, the grain interfaces are mostly modelled by zero-thickness cohesive elements which usually are based on a traction-separation relationship rather than a stress-strain relationship. On a cohesive interface, the traction at each point is considered as a function of the gap between the two sides of the crack (or displacement jump). Several mathematical models for traction-separation relationships have been proposed in the literature to represent failure in different materials, e.g. laminated composites Allix and Corigliano [4], concretes Wang [42] and polycrystalline materials Needleman [24], and Sfantos and Aliabadi [34]. Tvergaard and Hutchinson [39,40] proposed a cohesive interface law for modelling fracture in ductile materials. Another noteworthy cohesive interface model which has been widely used for the modelling of failure in polycrystalline materials is the potential-based cohesive law proposed by Xu and Needleman [44]. It has been employed extensively for modelling fracture in brittle materials, e.g. Shabir et al. [35]. For a comprehensive overview on cohesive interface models see Brocks et al. [7], Mosler [22].

Wei and Anand [43] developed a computational tool for an elasto-plastic interface model coupled with a crystal-plasticity model for the grain interior to investigate the deformation and

* Corresponding authors.
E-mail addresses: ahmad.akbari.r@iauksh.ac.ir, ahmad.akbari.r@gmail.com (A. Akbari), kerfridenp@cardiff.ac.uk (P. Kerfriden), stephane.bordas@alum.northwestern.edu (S. Bordas).

https://doi.org/10.1016/j.compstruc.2017.09.005
0045-7949/

fracture response of nanocrystalline nickel. They discussed the effect of the grain size on the macroscopic stress-strain curve, and it was concluded that the nanocrystalline nickel showed a brittle response when a high yield strength of the grain interiors and a relatively weaker strength of the interfaces is assumed. This means that inter-granular fracture can be assumed if grain boundaries are weaker than grain bodies.

Paggi and Wriggers studied inter-granular fracture using a non-local cohesive interface model with non-zero thickness interfaces. In their model, the thickness of the interfaces depend on the grain size. It should be emphasized that our approach will closely follow Paggi and Wriggers [29,30], who introduced a damage variable based on relative displacements in their cohesive zone model formulation. An atomistic approach was proposed in Glaessgen et al. [12] to study grain boundary fracture in polycrystalline aluminium. The constitutive model of the traction-separation relationship at the cohesive interfaces was characterised by a molecular-dynamics simulation of the physical behaviour at the nanoscale. Abdollahi and Arias [1] simulated the fracture processes of ferroelectric polycrystals in three dimensions using a phase-field model. In their model, the grain boundaries, cracks and the ferroelectric domain walls are represented in a diffuse way by three phase-fields, in order to avoid the difficulty of tracking the interfaces in three dimensions.

Recently, Mosler and Scheider [23] proposed a thermodynamically consistent cohesive model based on an energy potential which depends on some internal variables related to the deformation history of the interface in addition to the current displacement jump. Their model is based on the Helmholtz energy which is separated into different parts corresponding to different failure modes by applying the Coleman and Noll procedure. In their model, the dissipation of energy is related to an internal variable called the damage parameter, in accordance with the second law of thermodynamics.

As mentioned previously, we wish to study the effect of inter-granular cracking at the engineering scale, which cannot be done without up-scaling. Computational homogenisation is a robust technique that is used to obtain the average response of heterogeneous microstructures [13,25,33,3] on the mathematical side. Many efforts have been dedicated to find relationship between the microscopic material parameters and the macroscopic properties using computational homogenisation, e.g. Fish and Yu [11], Feyel and Chaboche [10], Kouznetsova [17], Hirschberg et al. [14], Talebi et al. [38], Silani et al. [36], and Jamshidian et al. [15,16]. However, the classic homogenisation scheme fails to characterise the overall response of a material in the softening regime Kouzbetsova [17], and this can be partially overcome, in specific situations, as shown in [26,27]. We limit our investigations to material states that remain macroscopically stable.

In this paper, a parameter study is performed to investigate the effect of cohesive inter-granular cracks on the overall macroscopical characteristics of polycrystalline microstructure under different quasi-static loading configurations. The quasi-static loading is applied by imposing Dirichlet boundary conditions on a two-dimensional non-regular representative volume element (RVE) of the polycrystalline microstructure, and a computational homogenisation technique is implemented. Two-dimensional grains are modelled as linear elastic materials, separated by cohesive interfaces under small strain condition. We perform several numerical experiments to understand the relationship between the microscopic parameters of the cohesive law, e.g. critical fracture energies in mode I and II, and the macroscopic material properties, e.g. stress–strain curve and yield surface. It will be shown that the computational homogenisation is capable to derive the macroscopic yield surface, provided that the microscopic parameters are given. This method is also can be used to charactrise the microscopic parameters when the macroscopic yield surface is available.

1.1. Outline

The paper is organized as follows. The next section presents a brief overview of the microscopic material model. In Section 3, the constitutive relationship for 2D orthotropic grains and the cohesive model for the interface between grains are explained. The finite element discretization and homogenisation scheme, the parametric studies of the cohesive law and their effects on the macroscopic behaviour of polycrystalline microstructure are reported in Section 4 which is followed by concluding remarks in the last section.

2. Micro-structural model formulation

Fig. 1 shows a domain Ω occupied by a structure consisting of randomly distributed orthotropic grains undergoing small quasi-static perturbations. The boundary value problem of a polycrystalline structure is detailed below.

Given the displacement boundary condition $\mathbf{u}_D : \partial\Omega_D \rightarrow \mathbb{R}^2$, find $\mathbf{u} : \Omega \rightarrow \mathbb{R}^2$ such that, $\forall \delta\mathbf{u} \in \mathcal{U}_0$

$$\delta\Pi(\mathbf{u}, \delta\mathbf{u}) = \int_{\Omega\setminus\Gamma} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\delta\mathbf{u}) \mathrm{d}\Omega + \int_{\Gamma} \mathbf{T} \cdot [\![\delta\mathbf{u}]\!] \mathrm{d}\Gamma - \int_{\partial\Omega_N} \mathbf{F} \cdot \delta\mathbf{u} \mathrm{d}\Gamma = 0 \tag{1}$$

$$(\boldsymbol{\sigma} \cdot \mathbf{n})|_{\mathbf{x}\in\Gamma^+} = -(\boldsymbol{\sigma} \cdot \mathbf{n})|_{\mathbf{x}\in\Gamma^-} = \mathbf{T}([\![\mathbf{u}]\!])|_{\mathbf{x}\in\Gamma}. \tag{2}$$

The vector $\mathbf{n}$ is a unit vector normal to the cohesive interface (see Fig. 2). $\delta\Pi$ is the virtual work, $\mathbf{u} \in \mathcal{U}$ is displacement field and $\delta\mathbf{u} \in \mathcal{U}_0$ is an arbitrary virtual displacement field. $\mathcal{U}$ and $\mathcal{U}_0$ are collections of trial, $\mathbf{u}$, and test functions, $\delta\mathbf{u}$ respectively, which can be defined by

$$\mathcal{U} = \{\mathbf{u} | \mathbf{u} \in H^1(\Omega \setminus \Gamma), \mathbf{u}|_{\partial\Omega_D} = \mathbf{u}_D\} \tag{3}$$

$$\mathcal{U}_0 = \{\delta\mathbf{u} | \delta\mathbf{u} \in H^1(\Omega \setminus \Gamma), \delta\mathbf{u}|_{\partial\Omega_D} = \mathbf{0}\} \tag{4}$$

where $H^1(\Omega \setminus \Gamma)$ is the broken Sobolev space of degree one in which the solution and trial functions associated with the interior of the grains, are sought.

The Cauchy stress tensor, the small strain tensor at the micro-scale are $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$, and the traction and displacement jumps on

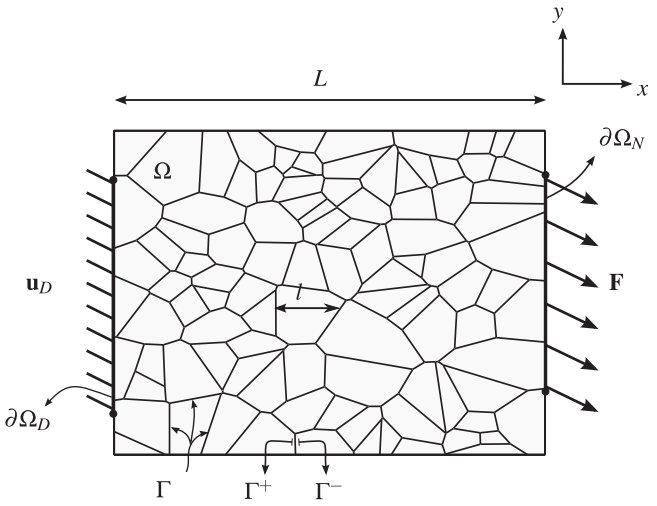

Fig. 1. A two-dimensional problem.

Please cite this article in press as: Akbari A et al. On the effect of grains interface parameters on the macroscopic properties of polycrystalline materials. Comput Struct (2017), https://doi.org/10.1016/j.compstruc.2017.09.005