Journal of the Mechanics and Physics of Solids 95 (2016) 374–392

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Homogenization of intergranular fracture towards a transient gradient damage model

G. Sun, L.H. Poh *

Department of Civil and Environmental Engineering, National University of Singapore 1 Engineering Drive 2, E1A-07-03, 117576, Singapore

A R T I C L E I N F O

Article history:
Received 5 December 2015
Received in revised form
15 April 2016
Accepted 17 May 2016
Available online 10 June 2016

Keywords:
A. Fracture
B. Crack mechanics
B. Constitutive behavior
B. Polycrystalline material
Homogenization theory

A B S T R A C T

This paper focuses on the intergranular fracture of polycrystalline materials, where a detailed model at the meso-scale is translated onto the macro-level through a proposed homogenization theory. The bottom-up strategy involves the introduction of an additional macro-kinematic field to characterize the average displacement jump within the unit cell. Together with the standard macro-strain field, the underlying processes are propagated onto the macro-scale by imposing the equivalence of power and energy at the two scales. The set of macro-governing equations and constitutive relations are next extracted naturally as per standard thermodynamics procedure. The resulting homogenized microforce balance recovers the so-called 'implicit' gradient expression with a transient nonlocal interaction. The homogenized gradient damage model is shown to fully regularize the softening behavior, i.e. the structural response is made mesh-independent, with the damage strain correctly localizing into a macroscopic crack, hence resolving the spurious damage growth observed in many conventional gradient damage models. Furthermore, the predictive capability of the homogenized model is demonstrated by benchmarking its solutions against reference meso-solutions, where a good match is obtained with minimal calibrations, for two different grain sizes.

1. Introduction

The analysis of material failure requires an efficient method to capture the propagation of underlying meso-scale processes onto the coarse engineering scale. In this paper, we focus on the brittle fracture of polycrystalline materials with intergranular cracks as the dominant failure mode, for instance in

- ceramics such as silicon carbide (e.g., Faber and Evans, 1983; Shih et al., 1998). Upon cooling from fabrication temperature, the built up of internal residual stresses due to the anisotropy of thermal expansion also induces intergranular fracture in ceramics (Rice and Pohanka, 1979);
- quenched and tempered alloy steels which have been heated in the range of 300–600 °C, or cooled slowly from the high temperature. Temper embrittlement is usually associated with fracture along prior austenitic grain boundaries, the degree of which increases with the concentration of intergranular impurities (e.g. Bandyopadhyay and McMahon, 1983; Banerji et al., 1978);

* Corresponding author.
E-mail address: ceeplh@nus.edu.sg (L.H. Poh).

http://dx.doi.org/10.1016/j.jmps.2016.05.035
0022-5096/

- degraded metallic materials due to hydrogen embrittlement in hostile environment, where fracture occurs along prior austenitic grain boundaries (e.g. McMahon, 2001; Pouillier et al., 2012).

A predictive failure analysis can be achieved by adopting a high resolution model with sub-granular discretization at the meso-scale, where interactions between different processes are directly accounted for. Yet, such a detailed modelling approach emanating from the meso-scale is seldom feasible for a typical engineering problem due to its inherent high computational cost. In the following, we confront this conundrum by developing a (lower resolution) macroscopically continuous model through a consistent homogenization theory, which retains a predictive capability comparable to that of a high resolution approach.

In general, the in-depth study on the brittle intergranular fracture of polycrystalline materials is an intricate issue, since the failure mechanisms transcend several length scales. At the initial stages of deformation, the nucleation and propagation of micro-cracks can be assumed to be uniformly distributed over the entire material. Beyond a certain threshold, the diffuse network of micro-cracks starts to coalesce into narrow region(s) and manifest themselves macroscopically as localized crack (s), the presence of which governs the overall structural response (Kraft et al., 2008). To directly capture the interactions between bulk material and micro-cracks in the numerical analyses of intergranular fracture, a natural approach is to have a sub-granular discretization of bulk material, with cohesive elements embedded at grain boundaries (e.g. An and Qin, 2013; Simonovski and Cizelj, 2013; Zhang et al., 2012). However, such a high resolution approach at the meso-scale is seldom practical for a typical engineering problem.

At the other end of the resolution spectrum, a continuum damage model disregards the underlying discreteness and solves for the overall behavior instead. Numerical analyses with standard models, however, become mesh dependent during strain softening. In the limit of vanishing element size, material failure occurs without any dissipation (Bazant and Jirasek, 2002). To this end, the so-called "implicit" gradient damage models have been developed, where an enriched variable and its gradient characterizing the underlying damage micro-processes are incorporated into the formulation (Peerlings et al., 1996). The length scale parameter associated with the higher order term, which is required for dimensional consistency, naturally characterizes the influence domain within which the micro-processes interact. Numerically, the length scale parameter serves as a localization limiter controlling the bandwidth of localized deformation, hence resolving the mesh dependency issue. In the literature, the implicit gradient enhancement has largely been interpreted as a reformulation of a nonlocal integral model, which incorporates the weighted average of the variable driving the damage process over an influence domain (e.g. Bazant and Pijaudier-Cabot, 1988; Comi, 2001; Pijaudier-Cabot and Bazant, 1987). Mathematically, it can be shown that an implicit gradient damage model bears a close resemblance, both in formulation and performance, to its nonlocal integral counterpart (Peerlings et al., 2001). Alternatively, an implicit gradient model can be developed from the micromorphic theory, where a "morphic" variable characterizing the damage micro-processes is incorporated into the thermodynamics framework of a generalized continuum (Forest, 2009; Dillard et al., 2006). Since these enriched continuum models do not explicitly resolve for the micro-processes, their numerical implementations permit a much coarser discretization than the underlying microstructures. This makes them computationally more amenable for practical usage.

Despite the general success of the implicit gradient enhancement in resolving the mesh dependency issue, many models in the literature suffer from the following limitations:

1. *Many assumptions and calibrations in phenomenological models*: The conventional approach in developing the nonlocal model is to adopt a "top-down" strategy, where macroscopic potentials and constitutive equations are postulated *a priori*. The accuracy of the model is thus constrained by the adequacy of postulations made. Moreover, the phenomenological models typically involve several parameters to be calibrated against reference data. Consequently, these models have limited predictive capabilities beyond the specific conditions or underlying microstructures which the modelling parameters are calibrated against.
2. *Partial regularization during strain softening*: Whereas the structural response is made mesh independent with the gradient enhancement, many models with a constant length scale parameter exhibit a spurious damage growth, where the damaged region expands with deformation instead of localizing into a macroscopic crack (Geers et al., 1998). This anomaly can be remedied by adopting a transient length scale parameter, where the interaction domain is made dependent on the level of underlying micro-cracks through the local strain field, such that a localized deformation is recovered at the final stage of loading (Geers et al., 1998; Saroukhani et al., 2013). A similar approach was adopted for an equivalent nonlocal integral formulation (Pijaudier-Cabot et al., 2004), motivated by a micro-mechanical analysis detailing the transient nature of interactions between micro-cracks. Alternative transient nonlocal interactions have also been formulated, e.g. by incorporating a length scale parameter that evolves with damage (Triantafyllou et al., 2014), by utilizing a damage dependent averaging of the local and nonlocal variables (Bui, 2010; Nguyen, 2011), or by adopting an interaction intensity based on the stress magnitude (Giry et al., 2011). While a transient nonlocal interaction fully regularizes the strain softening response, it requires additional constitutive assumptions and material parameters for the evolution of the length scale parameter, hence further undermining the predictiveness of the phenomenological model.

One strategy in addressing the above-mentioned limitations is to develop gradient damage models with suitable homogenization schemes, in order to extract constitutive laws and/or material parameters directly from the underlying microstructure. However, constructions of homogenized gradient/nonlocal damage models are rare in the literature. To