ARTICLE IN PRESS

Available online at www.sciencedirect.com

ScienceDirect

Comput. Methods Appl. Mech. Engrg. ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Computer methods in applied mechanics and engineering

www.elsevier.com/locate/cma

A non-isothermal thermodynamically consistent phase field framework for structural damage and fatigue

J.L. Boldrini[a], E.A. Barros de Moraes[b], L.R. Chiarelli[b], F.G. Fumes[b], M.L. Bittencourt[b],*

[a] *Department of Mathematics, Institute of Mathematics, Statistics and Scientific Computing, University of Campinas, SP, 13083-859, Brazil*
[b] *Department of Integrated Systems, School of Mechanical Engineering, University of Campinas, SP, 13083-970, Brazil*

Abstract

We present a general thermodynamically consistent non-isothermal non-local framework for the evolution of damage, fatigue and fracture in materials under the hypothesis of small deformation. The approach is based on the principle of virtual power (PVP), the balance of energy and the second law of thermodynamics in the form of the generalized Clausius–Duhem inequality for the entropy. In addition to the usual physical fields, the model uses the phase field approach to describe the evolution of both damage and fatigue. The kinematic descriptor (phase field) for damage is considered a continuous dynamical variable whose evolution equation is obtained by the PVP. The kinematic descriptor (another phase field) for fatigue is a continuous internal variable whose evolution equation is considered as a constitutive relation to be determined in a thermodynamically consistent way. The behavior of particular material classes can be specified by their corresponding free-energy potentials (which gives the reversible parts of the involved thermodynamic forces) and their associated pseudo-potentials of dissipation (which gives the irreversible parts of the involved thermodynamic forces). To exemplify our general framework, we present the case of an isotropic linear elastic material with viscous dissipation and constant specific heat. The corresponding case of irreversible damage is also presented by using penalization. The considered damage and fatigue phase field approach is a framework from which other methods in the literature may be recovered. The model is approximated by the nodal high-order finite element method with explicit fourth-order Runge–Kutta time integration. Results for one-dimensional examples are presented and conclusions are addressed.

Keywords: Damage; Fatigue; Phase field; Non-local model; Thermodynamically consistent model; High-order finite element method

---

1. Introduction

The understanding of damage evolution, fatigue and fracture in materials is very important in many engineering applications. Many researchers have contributed to several aspects to understand such phenomena and a significant amount of works can be found in the literature (e.g. Lemaitre and Desmorat [1], Kanninen and Popelar [2] and

---

* Corresponding author.
E-mail address: mlb@fem.unicamp.br (M.L. Bittencourt).

http://dx.doi.org/10.1016/j.cma.2016.08.030

Please cite this article in press as: J.L. Boldrini, et al., A non-isothermal thermodynamically consistent phase field framework for structural damage and fatigue, Comput. Methods Appl. Mech. Engrg. (2016), http://dx.doi.org/10.1016/j.cma.2016.08.030

Anderson [3]). However, some aspects of these phenomena are rather difficult to include in a phenomenological, thermodynamically consistent continuous model. For instance, crack initiation is one of these difficult aspects. A very challenging task nowadays is to develop consistent mathematical models that seamlessly describe initiation of damage and its evolution, fatigue and ultimately the fracture for different types of materials.

In recent years, more attention has been given to the phase field methodology as a promising way to deal with the modeling of material damage. Phase field models were originally developed to solve separation of fluids [4]. These models have been used in a great variety of multiphase problems such as in the study of tumor growth [5], vesicle-fluid iteration [6], solidification [7] and fluid–structure iteration problems [8]. Recently, phase field has gained large attention in modeling problems involving crack propagation, damage and fatigue which are major problems in many areas of engineering, physics and medicine. Thermodynamical consistency for damage and fatigue models are attempted by using the Ginsburg–Landau free-energy functional in order to predict the phase field evolution in continuum mechanics and solid materials [9–11].

The sharp interface between the material and void spaces is one of the main difficulties in modeling fractures. A continuum field model that capture crack initiation, propagation, dynamic fracture instability, sound emission, crack branching and fragmentation was presented in [12]. Another continuum model for mode III dynamic fracture based on phase field was used to simulate a two dimensional crack motion in a strip geometry above the Griffith threshold [13]. A quasi-static model is approximated by means of the Galerkin method using NURBS and T-spline basis functions in [14] as the finite dimensional approximation spaces for the weak form. Numerical results were presented with good agreement with experimental results. Phase field models have been extensively used to study quasi-static and dynamic fracture in brittle materials and the finite element approximation of these models is reviewed in [15]. Hybrid formulation which enables significant reduction of computational cost is proposed. The formulation is tested in several benchmark problems, including experimental verification.

A fourth-order phase field model for fracture based on local maximum entropy (LME) approximants is presented in [16]. With this numerical treatment, the expressions appearing in the Ritz–Galerkin variational formulation are easier to obtain and do not require different treatments such as in discontinuous Galerkin based methods. The model allows the use of highly non uniform meshes and local refinement. It is shown that the fourth-order model captures the crack surface more accurately and needs less nodes.

Crack propagation in multiphase systems is studied in [17] by using a combination of mechanical approach for the description of crack propagation with the multiphase-field model presented by [18]. Numerical simulations in transcrystalline as well as an intercrystalline materials show that the proposed model makes a large-scale simulation in multi-grain systems with the phase field method at all possible and also offers the possibility to investigate crack propagation and phase transformation process of solid phases simultaneously. Another work involving microstructures is presented in [19] where a formulation is developed within the phase field method for modeling interactions between interfacial damage and bulk brittle cracking in complex microstructures. The several benchmarks presented to validate the model show that the method captures nucleation from interfaces and propagation within the matrix, and for arbitrary geometries and interactions between cracks.

In [20], a phase field theory for fracture of nonlinear elastic materials is developed involving incremental minimization of a suitable free-energy functional. The Euler–Lagrange equations are incorporated to a fully three-dimensional anisotropic finite element implementation. The work apparently reports the first phase field theory of fracture accounting for simultaneous geometric nonlinearity, nonlinear elasticity and surface energy anisotropy. Some engineering brittle materials present ductile behavior after reaching the strength limit which creates a small-scale zone ahead the crack tip that exhibits growth and coalescence. This is caused by cohesive forces acting in the crack zone and a model for brittle and cohesive fracture is presented by [21] in order to predict this phenomenon. A geometric approach to diffusive crack modeling based on the introduction of a balance equation for a regularized crack surface is presented in [22] in order to model from brittle to ductile fracture coupled with thermo-plasticity at finite strains. Even with the continuous transition, the high gradient between the phases makes continuum formulations typically unable to describe crack propagation [23] and discrete methods such as finite element method (FEM) are usually used associated to techniques that capture [24] and treat discontinuities including remeshing [25] and embedding, such as the extended FEM (XFEM) [26].

However, the previously briefly described works have deficiencies. For instance, crack initialization is not usually considered, and so most of the known fracture models introduce some damage where the crack starts and then propagates through it; also, the thermodynamic consistency of some of the presented models is unclear, while others

Please cite this article in press as: J.L. Boldrini, et al., A non-isothermal thermodynamically consistent phase field framework for structural damage and fatigue, Comput. Methods Appl. Mech. Engrg. (2016), http://dx.doi.org/10.1016/j.cma.2016.08.030