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Thermal shock response via weakly coupled peridynamic thermo-mechanics

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ABSTRACT

A 3D peridynamic formulation of the thermo-mechanical problem allows to efficiently simulate the occurrence and propagation of cracks due to extreme thermal loading. The model is weakly coupled since no internal heat generation due to material deformation and damage is accounted for. As such, it is suitable to simulate low strain rate phenomena. Since the typical time scales of the mechanical and thermal systems may differ of several orders of magnitude, using a multirate explicit integration technique is suggested by the nature of the problem itself. Finally, the proposed formulation is used to model the thermal shock behavior of thin and thick slabs, in order to observe respectively a 2D ordered set of parallel cracks and a 3D honeycomb crack pattern addressed as columnar jointing.

1. Introduction

Most of the theories developed to simulate fracture nucleation and propagation are based on the local continuum theory. The effectiveness of standard finite elements for such problems is however severely impaired by the well-known mesh-dependency of the solution and the need to remesh the domain as the fracture propagates. Many numerical techniques have been developed so far in order to overcome some of the above mentioned shortcomings of the standard FEM; among them, the cohesive elements, meshless methods and the eXtended-FEM (X-FEM) are worth citing. Cohesive elements bypass the mesh-dependency problem by explicitly accounting for the finite dimension of the elements, thus allowing to account for a proper energy balance, as shown by e.g. Wells and Sluys (2001) and de Borst et al. (2004). Meshless methods allow to easily adapt the discretization in order to follow the crack tip, see e.g. Belytschko et al. (1996). This is often balanced by an increased overall complexity of the numerical formulation, as well summarized by Nguyen et al. (2008). The X-FEM allows to account for fracture propagation without the need to remesh the domain, see e.g. Moës and Belytschko (2002); similar, simplified techniques can be applied also to meshfree methods, as shown e.g. by Rabczuk and Belytschko (2004). The regularized variational formulation proposed by Bourdin et al. (2013) is also worth citing.

A completely different class of approaches for the study of fracture formation and propagation is based on the direct application of Newtonian mechanics. These techniques are based on networks of concentrated masses connected by springs, and have been used, among other things, to study columnar fracture process in granule-water mixtures (Nishimoto et al., 2007), crack propagation in crystals (Hayakawa, 1994a, 1994b), failure of brittle materials (Curtin and Scher, 1990) and composite materials transverse ply cracking Wittel et al. (2003).

The peridynamic (PD) theory, first proposed by Silling (2000), is a non-local formulation that allows to easily account for localization and fractures. Peridynamics has been successfully applied to the study of many problems, ranging from impact and/or penetration to crack propagation and bifurcation, dynamic fracture of membranes and mesoscale fracture modeling. Some noteworthy applications are shortly mentioned hereafter. Silling (2003) modeled the Kalthoff and Winkler (1988) experiment and correctly predicted the crack propagation angle in a notched plate made of maraging steel hit by a steel impactor. Later, Silling and Askari (2004) simulated the impact of a spherical, infinitely rigid projectile on an elastic-fragile thin disk. Demmie and Silling (2007) simulated structures under extreme loading conditions. Madenci and Oterkus (2016) developed a formulation to simulate plastic deformations based on von Mises yield criteria with isotropic hardening, while O'Grady and Foster (2014) addressed the bending of a Kirchhoff-Love plate.

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Thermal deformations have been taken into account in order to predict crack paths due to prescribed thermal temperature histories in the body. For example, Kilic and Madenci (2009) predicted complex crack growth patterns plates after quenching. More recently Amani et al. (2016) simulated the Taylor-bar impact, accounting for temperature change due to plastic dissipation, but completely neglecting thermal conduction thanks to the extremely short time of the impact.

Besides structural mechanics, PD has been used to develop complex models of multiphysics phenomena by e.g. Gerstle et al. (2007), where the thermal diffusion problem was reformulated for the first time using peridynamics. Later on, Bobaru and Duangpanya (2010, 2012) independently reformulated the heat equations in 1D and 2D, respectively. Their non-local solution tends to the local one as the coefficient that defines the material non-locality, addressed to as the horizon, tends to zero. Furthermore, Agwai (2011) proposed a PD formulation of the heat problem and a coupled formulation for the multiphysics thermo-mechanical problem and applied it to one dimensional elastic problems. Madenci and Oterkus (2014, Chapter 13) simulated two- and three-dimensional thermo-elastic problems. As a matter of fact, the PD reformulation of both the mechanical and the thermal problem presents some advantages, such as the possibility to use the same discretization to study both the mechanical and thermal transient problems and the capability of both models to take into account the onset of fracture surfaces during the simulation. However, none of the previous coupled thermo-mechanic papers did account for fractures; only very recently Oterkus and Madenci (2017) approached the coupled thermo-mechanic set of equations to simulate the thermal cracking of uranium dioxide fuel pellet.

This paper addresses the coupled PD thermo-mechanical problem in presence of evolving damages due to extreme thermal loading. Hence, the multiphysics thermo-mechanical problem is reformulated via PD, with the thermal-induced deformation affecting the mechanical response, and the onset of fracture surfaces preventing the transmission of heat. The formulation is implemented within the Open Source code Peridigm, see Park et al. (2012) for details.

The paper is organized as follows. The weakly coupled thermo-elastic peridynamics is briefly summarized in Section 2; due care is given to the definition of thermal boundary conditions, see Section 2.2. The thermal code is validated in Section 3. Finally, two thermo-mechanical crack problems are dealt with in Section 4.

2. Weakly coupled thermo-elastic peridynamics

The PD formulation of the fully coupled thermo-mechanics has been developed by Gerstle et al. (2007), and later by Agwai (2011) and Madenci and Oterkus (2014, Chapter 13). In their work Madenci and Oterkus provided also a non-dimensionalization of the equations and some benchmark tests, such as a semi-infinite bar under thermal loading, thermo-elastic vibrations of a bar and a block of material under thermal loading. Agwai (2011) and Madenci and Oterkus (2014) solved the coupled problems without considering the possibility of an evolving damage in the domain of interest. The three-dimensional formulation here proposed, instead, follows a slightly different approach. The thermal problem is reformulated similarly to what proposed by Bobaru and Duangpanya (2010, 2012). Additionally, weak coupling between the thermal and the mechanical problem is assumed, so that a variation of temperature may introduce a thermal loading in the structure, but a change of the loading conditions cannot cause a variation of temperature. This assumption is generally valid for brittle-elastic materials, such as ceramics. This is the reason for which the case studies addressed in this paper simulate the behavior of alumina samples. A damage model based on the critical stretch criterion is introduced in the equations. This allows to properly account for material failure.

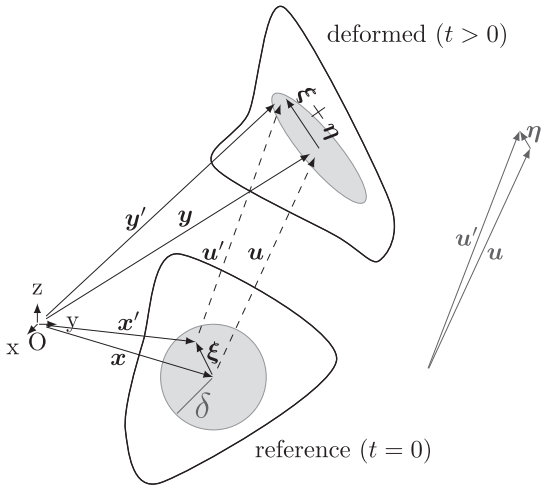

Fig. 1. Kinematics in the reference and deformed configurations for a PD continuum.

The following section briefly summarizes the weakly-coupled thermo-elastic peridynamic theory. It is by no means intended to be an exhaustive introduction to peridynamics; many results are reported without the corresponding proofs, that can be found in the cited references. Note also that even the notation developed throughout the years for the peridynamic theory is somewhat different from that of classical continuum mechanics. Notwithstanding our effort to be accurate and self-contained, the reader not accustomed to peridynamics is thus encouraged to refer to Silling et al. (2007), Silling (2010) and Silling and Lehoucq (2010) for a thorough introduction.

2.1. Governing equations

The peridynamic formulation that was first proposed is called bond-based peridynamics (BB-PD). It defines the density $\boldsymbol{f}$ of internal (bond) forces per unit of volume which are exchanged between different material points within a continuum. Thus, material points interact through bonds, with bond force densities depending only on the two interacting material points. Bonds forces are assumed to be non null only within a finite distance δ addressed as horizon. The horizon is a material constant, and directly defines the material non-locality (see Ren et al. (2016) for an improved formulation with variable horizon). Note that $\boldsymbol{f}$, often referred as bond forces, are actually density of forces per unit of volume, i.e. forces per unit of volume squared. The force per unit of volume applied at any given point $\boldsymbol{x}$ is thus given by the integral, performed over the volume defined by the horizon, of the bond forces. The resulting equation of motion is thus

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\mathfrak{S}_\delta} \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{x}',t) - \boldsymbol{u}(\boldsymbol{x},t), \boldsymbol{x}' - \boldsymbol{x}) \mathrm{d}V_{\boldsymbol{x}'} + \boldsymbol{b}(\boldsymbol{x},t) \qquad (1)$$

with ρ the material density, $\boldsymbol{u}$ the displacement, $\boldsymbol{b}$ the applied forces per unit of volume and $\mathfrak{S}_\delta$ the sphere of radius δ centered in $\boldsymbol{x}$; $\mathrm{d}V_{\boldsymbol{x}'}$ means that the integral is performed over $\mathfrak{S}_\delta$ by keeping $\boldsymbol{x}$ fixed and varying $\boldsymbol{x}'$. The relative position of two points in the reference configuration is often referred as $\boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$; their relative displacement is $\boldsymbol{\eta} = \boldsymbol{u}' - \boldsymbol{u}$, so that their relative position in the deformed configuration is $\boldsymbol{y}' - \boldsymbol{y} = \boldsymbol{\xi} + \boldsymbol{\eta}$, cfr. Fig. 1. Silling (2000) showed that, for a microelastic brittle BB-PD ma-