THERMODYNAMICAL ASPECTS OF IMPLICIT GRADIENT DAMAGE

R.H.J. PEERLINGS & M.G.D. GEERS
Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

ABSTRACT

A gradient damage formulation for quasi-brittle damage is derived from a nonstandard expression for the free energy potential. In contrast with many existing approaches, the nonstandard terms are related to the kinematics of the problem and therefore come into play already in the elastic regime. Following the argument that the second law of thermodynamics need only be satisfied globally for a nonlocal continuum, an energy balance equation is derived which must be solved together with the usual equilibrium equations. Numerical solutions of this coupled set of equations have been generated for a one-dimensional problem in order to study the localisation behaviour of the formulation. In the limit where the elastic modulus related to the energy balance goes to zero, an earlier gradient damage model is retrieved.

1 INTRODUCTION

The degradation and fracture of concrete, ceramics, fibre-reinforced polymers and other quasi-brittle materials can be successfully modelled using nonlocal and gradient damage theories. The presence of some form of nonlocality in these theories is crucial in avoiding pathological localisation effects. The nonlocality can take the form of integral relations between the internal variables of the theory, as first proposed by Pijaudier-Cabot and Bažant [1], or of gradients of internal variables or strain, a suggested in plasticity by Aifantis [2]. Theories of the latter class are usually weakly nonlocal. This means that the spatial interactions provided by them are limited to infinitesimal distances. Theoretical arguments and numerical solutions suggest that this type of nonlocality may be too weak to eliminate pathological localisation effects in the limit of complete failure of the material [3]. Integral formulations are strongly nonlocal by definition and therefore do not suffer from this shortcoming. However, they lead to governing equations which are of the integro-differential type and which do not fit very well in the classical framework of nonlinear computational mechanics. The so-called implicit gradient damage formulation proposed by Peerlings et al. [4] eliminates this disadvantage. It replaces the spatial averaging used in the integral formulation by a partial differential equation which must be solved simultaneously with the partial differential equations which describe equilibrium. Although the resulting theory has some similarity with the gradient theories indicated above, it can be shown to provide strong nonlocality [5] and has been used successfully to model quasi-brittle fracture, see e.g. refs [6, 7].

Although it can be motivated heuristically by micromechanical arguments, the physical implications of the additional partial differential equation which enters the implicit gradient theory is not immediately clear. This becomes particularly apparent in the boundary conditions which must accompany it, and for which a rigorous physical interpretation has been missing. This paper is an attempt to partially fill this gap. It draws on ideas put forward by, among others, Svedberg and Runesson [8], Polizzotto and Borino [9], Lorentz and Andrieux [10] and Liebe et al. [11], who proposed thermodynamical frameworks for nonlocal and gradient formulations in plasticity and

damage. Common to these theories is the notion that nonlocality allows the direct and instantaneous exchange of energy within the continuum. As a consequence of these energy exchanges, the Clausius-Duhem inequality may no longer be satisfied in its classical, pointwise form. Requiring it to hold globally, for the entire body, then allows to construct equations which govern the nonlocal energy transfer. Following this strategy for a particular form of the free energy function, an implicit gradient damage theory can be derived which is very similar to that of ref [4]. It will be shown that exactly this theory can be recovered as a limit case. The nonstandard partial differential equation of the original theory is obtained as a natural outcome, and the boundary conditions associated with it get a clear physical interpretation in terms of energy flow.

2 THERMODYNAMICAL BASIS

As a starting point of our development we postulate a Helmholtz free energy functional of the form

$$\psi(\boldsymbol{\varepsilon}, \tilde{\varepsilon}, \bar{\varepsilon}, D) = \tfrac{1}{2}(1-D)\,\boldsymbol{\varepsilon}:\boldsymbol{C}:\boldsymbol{\varepsilon} + \tfrac{1}{2}h(\tilde{\varepsilon}-\bar{\varepsilon})^2 + \tfrac{1}{2}hl^2\|\vec{\nabla}\bar{\varepsilon}\|^2. \tag{1}$$

The first term in this expression is classical in damage mechanics. In it, $\boldsymbol{\varepsilon}$ denotes the linear strain tensor and $\boldsymbol{C}$ is the (undamaged) elasticity tensor; the isotropic damage variable D degrades the elastic stiffness. In the second and third terms of (1), $\tilde{\varepsilon}$ is a scalar invariant of the strain tensor which is relevant in terms of the degradation process, see e.g. [6], whereas $\bar{\varepsilon}$ is at this stage considered as an independent field variable and is termed nonlocal strain. It can be immediately seen from (1) that differences between $\tilde{\varepsilon}$ and $\bar{\varepsilon}$ as well as gradients of $\bar{\varepsilon}$ are penalised and that $\bar{\varepsilon}$ will thus tend to be smoother than $\tilde{\varepsilon}$. The parameters h and l, which govern the relevance of the nonstandard terms, are positive and have the same dimension as Young's modulus and the dimension of length respectively.

Expression (1) differs from earlier proposals by Lorentz and Andrieux [10] as well as Liebe et al. [11] on two important aspects. Firstly, the nonstandard quantity $\bar{\varepsilon}$ which, as we will see below, carries the nonlocal interactions, is not attached to an internal variable of the damage influence, but is a 'deformation-like' variable, although it is not directly linked to the kinematics. And secondly, partially as a consequence of this relation to the deformation, $\bar{\varepsilon}$ and the nonlocality described by it are active in the entire body, even in those parts in which no damage has occurred yet. This contrasts with the gradient of damage used in refs [10] and [11], which evolves only in the process zone where damage grows. It should also be mentioned that, unlike for instance Benvenuti et al. [12], we do not define the relation between $\tilde{\varepsilon}$ and $\bar{\varepsilon}$ a priori. On the contrary, this relationship and the precise role played by $\bar{\varepsilon}$ will emerge as a result of our development.

Using the free energy potential according to (1), the constitutive relations can now be developed by considering the global Clausius-Duhem dissipation inequality

$$\dot{\mathcal{D}} := \int_V \left(\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}} - \dot{\psi}\right) \mathrm{d}V \geq 0. \tag{2}$$

Note that in accordance with the statements made above, the integration involves the entire body volume V and not only the process zone. Differentiation of (1) with respect to time and substitution into (2) yields

$$\dot{\mathcal{D}} = \int_V \left[\boldsymbol{\sigma} - (1-D)\,\boldsymbol{C}:\boldsymbol{\varepsilon} - h(\tilde{\varepsilon}-\bar{\varepsilon})\boldsymbol{N}\right]:\dot{\boldsymbol{\varepsilon}}\;\mathrm{d}V + \int_V \left[h(\tilde{\varepsilon}-\bar{\varepsilon})\,\dot{\tilde{\varepsilon}} - hl^2\vec{\nabla}\bar{\varepsilon}\cdot\vec{\nabla}\dot{\bar{\varepsilon}}\right]\mathrm{d}V + \int_V \tfrac{1}{2}\,\boldsymbol{\varepsilon}:\boldsymbol{C}:\boldsymbol{\varepsilon}\,\dot{D}\;\mathrm{d}V, \tag{3}$$

where $\boldsymbol{N} = \partial\tilde{\varepsilon}/\partial\boldsymbol{\varepsilon}$. Since the $\bar{\varepsilon}$ and $\vec{\nabla}\bar{\varepsilon}$ fields cannot be varied independently, the term involving the latter quantity is integrated by parts, resulting in

$$\dot{\mathcal{D}} = \int_V \left[\boldsymbol{\sigma} - (1-D)\,\boldsymbol{C}:\boldsymbol{\varepsilon} - h(\tilde{\varepsilon}-\bar{\varepsilon})\boldsymbol{N}\right]:\dot{\boldsymbol{\varepsilon}}\;\mathrm{d}V + \int_V h\left[\tilde{\varepsilon}-\bar{\varepsilon}+l^2\nabla^2\bar{\varepsilon}\right]\dot{\tilde{\varepsilon}}\;\mathrm{d}V$$
$$- \int_S hl^2\vec{\nabla}\bar{\varepsilon}\cdot\vec{n}\;\dot{\tilde{\varepsilon}}\;\mathrm{d}S + \int_V \tfrac{1}{2}\,\boldsymbol{\varepsilon}:\boldsymbol{C}:\boldsymbol{\varepsilon}\;\dot{D}\;\mathrm{d}V, \quad (4)$$

where S denotes the boundary of V and $\vec{n}$ is the outward unit normal to S.

Now following the usual arguments the first integral vanishes by assuming the stress-strain relation

$$\boldsymbol{\sigma} = (1-D)\,\boldsymbol{C}:\boldsymbol{\varepsilon} + h(\tilde{\varepsilon}-\bar{\varepsilon})\boldsymbol{N}. \quad (5)$$

The first term of this relation is classical; the second is not and is related to the nonlocality. Note that, contrary to most nonlocal and gradient damage theories, this nonlocal contribution is active already in the elastic regime, before any damage has developed. Accordingly, the elastic behaviour of the present formulation will deviate from standard linear elasticity. When there is no damage growth, i.e. when $\dot{D} = 0$ in V, the last integral in (4) also vanishes. In this case the behaviour of the model should be elastic and we should thus have $\dot{\mathcal{D}} = 0$. The following conditions are sufficient for this to hold:

$$h\left[\tilde{\varepsilon}-\bar{\varepsilon}+l^2\nabla^2\bar{\varepsilon}\right] = 0 \qquad \text{in } V, \quad (6)$$

$$hl^2\vec{\nabla}\bar{\varepsilon}\cdot\vec{n} = 0 \qquad \text{on } S. \quad (7)$$

These equations form a boundary value problem in terms of the nonlocal equivalent strain $\bar{\varepsilon}$ which must be solved together with the standard equilibrium equations. The two sets of equations are mutually coupled through the appearance of $\tilde{\varepsilon}$ in (6) and of $\bar{\varepsilon}$ in (5). Physically, eqn (6) determines the amount of energy which is available for nonlocal energy exchanges within the body. It is emphasised that this equation must hold on the entire domain V, i.e. in elastic regions as well as in possible process zones, and that energy may thus also be exchanged between elastic and damaging material. Eqn (7) expresses that there can be no energy exchange across the boundary as a result of the nonlocality, cf. the insulation condition of Polizzotto and Borino [9]. Note that (7) must be applied at the external boundary of the body and not at the boundary of the process zone, which is a considerable advantage in numerical implementations since the process zone will generally change in time.

Having established the nonstandard balance equations (6)–(7), the dissipation inequality can finally be written as

$$\dot{\mathcal{D}} = \int_V Y\dot{D}\;\mathrm{d}V \geq 0, \quad (8)$$

where the damage energy release rate has been defined as

$$Y = \tfrac{1}{2}\,\boldsymbol{\varepsilon}:\boldsymbol{C}:\boldsymbol{\varepsilon}. \quad (9)$$

Given the fact that $Y \geq 0$, the usual condition that damage can only increase, i.e. $\dot{D} \geq 0$, is sufficient for (8) to hold. In the absence of damage growth, no dissipation is taking place and eqns (5)–(7) can be regarded as an implicit gradient elasticity model.

Following our earlier work, the limit of the elastic regime is defined here in terms of the nonlocal equivalent strain by assuming the following damage criterion [4]:

$$f(\bar{\varepsilon}, \kappa) = \bar{\varepsilon} - \kappa \leq 0. \tag{10}$$

Damage can grow only if the equality sign holds and remains constant for $f < 0$. The history variable κ follows from the Kuhn-Tucker relations

$$f \leq 0, \qquad \dot{\kappa} \geq 0, \qquad f\dot{\kappa} = 0 \tag{11}$$

and an initial value $\kappa|_{t=0} = \kappa_0$ which indicates the initial elastic domain. It can easily be seen that κ is always equal to the highest $\bar{\varepsilon}$ experienced locally during the loading history – or to the initial value κ_0 if this value has not been reached yet. Since κ can never decrease, the damage variable can be related directly to it: $D = D(\kappa)$. Consequently, nonlocal energy exchanges either contribute to the growth of damage or to the increase of elastically stored energy elsewhere.

3 LOCALISATION BEHAVIOUR AND COMPARISON WITH EARLIER THEORY

In order to study the localisation behaviour of the damage model developed above, numerical solutions have been generated for a one-dimensional problem which was used before in ref [4] and elsewhere. We consider a bar of length 100 mm and a uniform cross section, except for a 10 mm zone in the centre, where the cross section area has been reduced by 10% in order to trigger localisation. Young's modulus of the material is taken to be $E = 20\,000$ MPa and in the reference computation the higher-order modulus h is set equal to E. The length parameter is $l = 1$ mm. The equivalent strain is set equal to the axial strain, and the damage evolution law is defined such that it results in linear softening in the uniform case, see ref [4] for details and parameter values. A uniform finite element discretisation of 200 elements has been used, with a quadratic interpolation of the displacement and a linear interpolation of the nonlocal equivalent strain. The computation was controlled using an indirect displacement control method combined with an automatic stepsize selection.

Fig 1 shows the distribution of the strain and nonlocal strain at several stages of the computation for the reference case where $h = E$. The gradient terms in the constitutive model clearly lead to

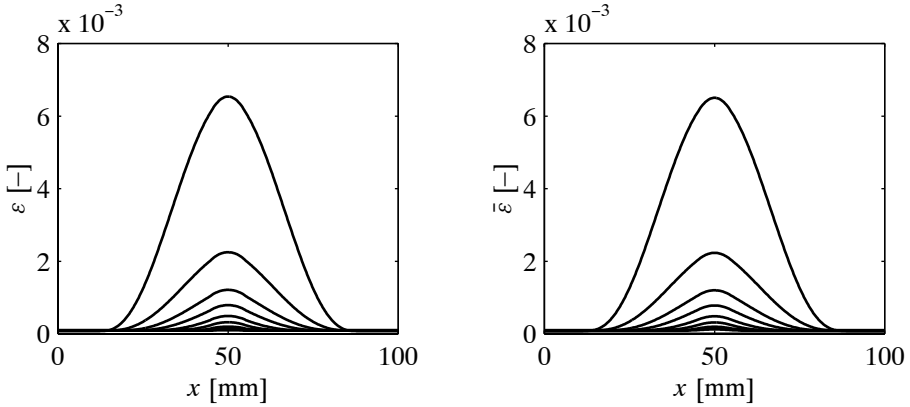

Figure 1: Evolution of the local strain (left) and nonlocal strain (right) for $h = E$

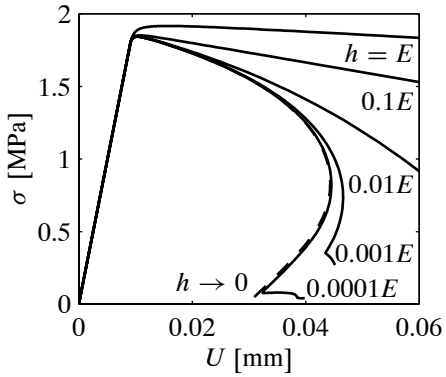

Figure 2: Stress in the bar vs end displacement for a range of higher-order moduli h; the dashed curve represents the simplified model of ref [4]

the development of a relatively wide band of intense deformation, rather than the localised solution within the imperfection that would occur without these terms. It is interesting to note that there is very little difference between the strain ε and the nonlocal strain $\bar{\varepsilon}$. The relatively high value of h clearly forces these fields together. For lower values of h, the difference between ε and $\bar{\varepsilon}$ indeed becomes more pronounced and the strain distribution is more localised.

Fig 2 shows the load-displacement curve obtained in the reference computation, as well as for decreasing values of h. The dashed curve in this diagram ($h \to 0$) has been obtained using our earlier theory as described in ref [4]. The response of the present, thermodynamically consistent gradient formulation clearly approaches this curve as h is diminished. This can be understood as follows. For any positive h and l, eqns (6)–(7) can be divided by h and hl^2 respectively. The resulting equations are exactly the same as those proposed in [4]. The only difference between the theory described in [4] and the present theory is therefore the nonlocal contribution to the stresses, i.e. the last, nonstandard term in eqn (5). If we now consider the limit $h \to 0$ and assume that the difference between the local and nonlocal equivalent strains remains finite, this term disappears and the stress-strain relation of [4] is thus retrieved. Physically, taking the limit $h \to 0$ can be interpreted as gradually 'switching off' any nonlocal effects in the elastic regime, while preserving the ability of the elastic region to influence damage growth in the process zone. It can easily be verified that the simpler theory which is thus obtained satisfies the energy balance and the dissipation inequality and is therefore also thermodynamically admissible.

4 CONCLUDING REMARKS

We have shown that a theory which is very similar to our earlier proposal in [4] may be derived via thermodynamical principles if a very specific form of the free energy potential is assumed. In the limit where the nonstandard modulus h vanishes, this theory reduces to the one proposed in [4]. The thermodynamical basis which has thus been given to this theory provides a clearer physical interpretation of the equations which govern its spatial interactions. The nonstandard partial differential equation (6) describes instantaneous energy transfer between material points (at a length scale given by l), whereas the boundary condition (7) inhibits such a transfer across the boundary of the body.

In its full form as developed here – i.e. for finite h – the theory still shows some shortcomings when pushed to the limit of complete fracture ($D \to 1$). In particular, some residual strength remains

in this limit (fig 2), whereas damage models classically predict vanishing stresses for $D = 1$. Related to this, the free energy does not go to zero in this limit. Both effects are caused by the fact that the terms that have been added to the free energy in order to describe nonlocal interactions do not depend on the damage variable. In reality, it can be very well imagined that the development of damage influences – or more specifically: degrades – the ability to relay energy fluxes. However, in the limit $h \to 0$ these effects vanish and the simplified formulation which may be obtained in this limit does not suffer from them. We believe that this theory allows to capture the most essential nonlocal mechanism in a way motivated by the full model and may therefore yield realistic results in many practical cases.

REFERENCES

[1] Pijaudier-Cabot G., Bažant Z.P. Nonlocal damage theory. Journal of Engineering Mechanics, 113, 1512–1533, 1987.

[2] Aifantis E.C. On the microstructural origin of certain inelastic models. Journal of Engineering Materials and Technology, 106, 326–330, 1984.

[3] Peerlings R.H.J., de Borst R., Brekelmans W.A.M., Geers M.G.D. Localisation issues in local and nonlocal continuum approaches to fracture. European Journal of Mechanics A/Solids, 21, 175–189, 2002.

[4] Peerlings R.H.J., de Borst R., Brekelmans W.A.M., de Vree J.H.P. Gradient-enhanced damage for quasi-brittle materials. International Journal for Numerical Methods in Engineering, 39, 3391–3403, 1996.

[5] Peerlings R.H.J., Geers M.G.D., de Borst R., Brekelmans W.A.M. A critical comparison of nonlocal and gradient-enhanced softening continua. International Journal of Solids and Structures, 38, 7723–7746, 2001.

[6] Peerlings R.H.J., de Borst R., Brekelmans W.A.M., Geers M.G.D. Gradient-enhanced damage modelling of concrete fracture. Mechanics of Cohesive-Frictional Materials, 3, 323–342, 1998.

[7] Geers M.G.D., de Borst R., Peerlings R.H.J. Damage and crack modeling in single-edge and double-edge notched concrete beams. Engineering Fracture Mechanics, 65, 247–261, 2000.

[8] Svedberg T., Runesson K. A thermodynamically consistent theory of gradient-regularized plasticity coupled to damage. International Journal of Plasticity, 13, 669–696, 1997.

[9] Polizzotto C., Borino G. A thermodynamics-based formulation of gradient-dependent plasticity. European Journal of Mechanics A/Solids, 17, 741–761, 1998.

[10] Lorentz E., Andrieux S. A variational formulation for nonlocal damage models. International Journal of Plasticity, 15, 119–138, 1999.

[11] Liebe T., Steinmann P., Benallal A. Theoretical and computational aspects of a thermodynamically consistent framework for geometrically linear gradient damage. Computer Methods in Applied Mechanics and Engineering, 190, 6555–6576, 2001.

[12] Benvenuti E., Borino G., Tralli A. A thermodynamically consistent nonlocal formulation for damaging materials. European Journal of Mechanics A/Solids, 21, 535–553, 2002.