Thermodynamic Derivation and Damage Evolution for a Fractional Cohesive Zone Model

Giulio Alfano, Ph.D.[1]; and Marco Musto, Ph.D.[2]

Abstract: A thermodynamic derivation is presented for a fractional rate-dependent cohesive zone model recently proposed by the authors to combine damage and linear viscoelasticity. In this setting, the assumptions behind the initially proposed damage evolution law are revisited. In particular, in the original model damage evolution is driven only by the energy stored in the elastic arm of a fractional standard linear solid model and the relationship between total fracture energy and crack speed is monotonically increasing, with a sigmoidal shape. Here, physical arguments are discussed, which could support the hypothesis of allowing damage to be driven also by the remaining parts of the free energy. The implications of these different assumptions are then studied, analytically and numerically, and in both cases the assumption that damage is also driven by the remaining parts of the energy results in a nonmonotonic relationship between total fracture energy and crack speed, with a bell rather than sigmoidal shape. The analysis presented provides a novel physical interpretation of the significant differences found in the rate dependence of fracture in elastomers and glassy polymers. **DOI: 10.1061/(ASCE)EM.1943-7889.0001203.**

Introduction

Rate dependence of fracture can be important in many engineering applications (Xu et al. 2003; Karac et al. 2011; Chan and Siegmund 2004; Oldfield et al. 2013). It can been investigated via "conventional" fracture mechanics, by assuming that fracture energy G_c is a function of crack speed $\dot{a}$—that is, $G_c = \gamma(\dot{a})$. However, this approach is rather phenomenological, which leads, first, to the requirement for a large number of experimental tests to identify the model parameters and, second, to the difficulty of extending the validity of these models outside the range of conditions within which tests have been conducted.

As an alternative method, cohesive zone models (CZMs) are increasingly been used to model fracture. In particular, a number of rate-dependent CZMs have been proposed (see Musto and Alfano 2013, 2015; Musto 2014 and references therein for a review of different approaches and models in the literature). In fact, CZMs and fracture mechanics can be treated with a unified approach within the framework of the variational theory of fracture (Bourdin et al. 2008). The reader is referred to Del Piero (2014) for a summary of recent developments, which are, however, limited to the rate-independent case.

When the rate dependence of fracture is mainly the result of the viscoelastic response of the material across the interface along which the crack propagates, the CZMs proposed in Musto and Alfano (2013, 2015) can be used. Common to both models is the idea that the energy dissipated during the fracture process is the combination of two different types of dissipation mechanisms, one associated with the "rupture" of elastic bonds (i.e., decohesion) and another one associated with viscous flow. Accordingly, by formulating the model within the framework of thermodynamics with internal variables, two different internal variables are introduced and associated with these different dissipation mechanisms: a damage parameter D to model the degree of decohesion and a "viscous" (Musto and Alfano 2013) or "elastoviscous" (Musto and Alfano 2015) part α of the relative displacement to model the viscous behavior. The term "elastoviscous" is borrowed from Deseri et al. (2014), as discussed later in more detail.

The second assumption made in Musto and Alfano (2013, 2015) is that decohesion is rate independent, whereby a rate-independent law is defined for the evolution of D. The rate dependence of the overall interface response is therefore the result of the viscous dissipative mechanism introduced in the model. In Musto and Alfano (2013), viscous dissipation is a quadratic function of $\dot{\alpha}$ and, in the absence of damage, the interface response is that of a viscoelastic standard linear solid (SLS) model. In this way, in the general case the interface stress is the product of a Volterra convolution operator, with exponential kernel, and a scaling factor $1 - D$, which accounts for interface damage. For a simple proof of concept the model in Musto and Alfano (2013) is kept to the simplest level so that a single relaxation time is considered, whereby the rate dependence of the response can be captured only over a limited range of crack speeds.

To increase the prediction capability of the model presented in Musto and Alfano (2013), one could simply increase the number of Maxwell arms of the rheological model, but this requires the calculation of a large number of constants. On the other hand, following the work of Nutting (1921), it is widely accepted that the behavior of most rate-dependent materials is captured with much better approximation if the exponential kernel in the Volterra convolution operator is replaced with a power-law kernel, at least within limited values of stresses and strains whereby linear viscoelasticity is a valid theory for the undamaged material. It has also been well known for almost 80 years (Scott Blair 1947) that the use of a power-law kernel is equivalent to the introduction of fractional derivatives when the problem is written in differential form, which has led to the development of fractional viscoelasticity.

[1]Dept. of Mechanical, Aerospace and Civil Engineering, Brunel Univ., Kingston Ln., Uxbridge UB8 3PH, U.K. (corresponding author). ORCID: http://orcid.org/0000-0002-8415-4589. E-mail: giulio.alfano@brunel.ac.uk

[2]Dept. of Mechanical, Aerospace and Civil Engineering, Brunel Univ., Kingston Ln., Uxbridge UB8 3PH, U.K. E-mail: marco.musto@brunel.ac.uk

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Based on these considerations, the model initially proposed in Musto and Alfano (2013) was refined in Musto and Alfano (2015) by considering a fractional viscoelastic model for the undamaged response. In particular, a "fractional" SLS (FSLS) model is used by replacing the dashpot of the SLS model used in Musto and Alfano (2013) with a new "Scott Blair element," in which the stress is proportional to the fractional derivative of order ν of the relative displacement, with $0 < \nu < 1$. This element was called a "spring-pot" in Musto and Alfano (2015), following (Koeller 1984), although here, following (Mainardi and Gorenflo 2007), it will be called the "Scott Blair element" to give credit to the pioneering work of G. W. Scott Blair, who was the first to introduce this constitutive law and the use of fractional derivatives to model a mechanical response that is intermediate between the two limit cases of a Hookean solid ($\nu = 0$) and a Newtonian fluid ($\nu = 1$).

The modification made in Musto and Alfano (2015) made the CZM capable of capturing the rate dependence of crack propagation across a rubber interface between the two steel arms of a double cantilever beam (DCB), with excellent approximation across the entire range of experimentally tested speeds, spanning almost 5 logarithmic decades, and with only 7 parameters to be calibrated. In particular, the model captures the experimentally measured monotonic increase in fracture energy over the tested range of speeds. Further numerical simulations of the pointwise response show that the fracture energy G_c predicted by the model is indeed monotonically increasing with the prescribed relative-displacement speed v, with horizontal asymptotes in the slow and fast limits. This results in a sigmoidal shape of the $G_c - v$ curve.

The aim of this paper is to revisit the third assumption that is made in both models proposed in Musto and Alfano (2013, 2015), whereby damage evolution is "driven" by the energy stored in the elastic arm of either the SLS model (Musto and Alfano 2013) or the FSLS model (Musto and Alfano 2015). One motivation for revisiting this hypothesis is that, for some glassy polymers (i.e., used below the glass-transition temperature) it is experimentally found that fracture energy does not increase monotonically with crack speed. In fact, it can be seen that if damage evolution is driven not only by the energy in the elastic arm but also by some or the entirety of the energy within the inelastic arm, the monotonicity of the $G_c - \dot{a}$ relationship can be lost. This is discussed in detail in the paper, and some physical arguments are used to justify the validity of this alternative modeling choice.

To better achieve the stated aim, a thermodynamic formulation of the CZM is also presented. To this end, because attention is here limited to isothermal processes, the (specific) free energy at an interface material point needs to be defined. However, for a general linear viscoelastic model governed by Volterra integral operators, the definition of free energy is not unique (Breuer and Onat 1964), unless a specific mechanical model is considered. This problem has been widely studied—for example, by enlarging the space of strain histories and processes and weakening requirements on their regularity. This allows for broadening the set of available free energies (e.g., Del Piero and Deseri 1996, 1997; Deseri et al. 1999; Fabrizio and Golden 2002). Such enlarged sets owe the lowest minimal free energy (e.g., Deseri et al. 1999, 2006; Amendola et al. 2016; Golden 2016 among many others), whereas the maximal one has been found to be the relaxed work performed by the stress on the available processes, as shown by Del Piero (2004).

The nonuniqueness of the free energy is a kernel-independent issue and so also applies to the fractional CZM proposed by Musto and Alfano (2015). When an exponential kernel is used, well-known rheological representations are available based on suitable combination of springs and dashpots, typically an elastic arm in parallel with a number of Maxwell arms, and the free energy can be easily evaluated as the elastic energy stored in the springs. For a fractional model, even if a rheological analogue is used by replacing dashpots with Scott Blair elements, such as in Musto and Alfano (2015), there is no clear separation between elastic (Hookean solid) and viscous (fluid) behavior in the latter. Here, an expression is used for the free energy of the Scott Blair element, which can be derived from a widely used general formula valid for generic relaxation functions in viscoelasticity (Staverman and Schwarzl 1952; Bland 1960; Hunter 1961; see also the analysis of macroscopic dissipation and free energies for power-law materials in Fabrizio 2014). In Deseri et al. (2014) it is shown that this expression is valid for a rheological analogue of the Scott Blair element previously introduced by Di Paola and Zingales (2012), who, building on earlier work by Bagley and Torvik (1983) and Schiessel and Blumen (1993, 1995), defined a general mechanical analogue that distinguishes "elastoviscous" behavior, for the fractional exponent $0 < \nu < 1/2$, from "viscoelastic" behavior, for $1/2 \leq \nu < 1$.

The structure of the paper is as follows. In a first section, the main equations governing the fractional CZM presented by Musto and Alfano (2015) are recalled. In the second section, a thermodynamic formulation of the model is presented. A number of possible damage evolution laws are then considered, first by considering micromechanical arguments in their support and then by reporting the actual equations that implement them within the CZM formulation. Numerical results are then presented to show the implications of different model choices and the sensitivity of the results to the fractional exponent ν. Finally, conclusions are drawn and the future outlook is discussed.

Formulation of the CZM

The paper focuses on Mode-I (opening) decohesion problems, in which a crack is expected to form and/or propagate across a predefined interface $\mathcal{I}$. The displacement field is allowed to be discontinuous on $\mathcal{I}$, and the opening relative-displacement component, normal to $\mathcal{I}$, is denoted δ. For simplicity, and without loss of generality, a process in which both stresses and displacements are zero for negative times is considered.

The rate-dependent CZM formulated in Musto and Alfano (2015), whose governing equations are recalled in this section, provides the normal interface stress at time t, $\sigma(t)$, as the following nonlinear functional of the relative-displacement history $\delta{:}[0, t] \rightarrow \mathfrak{R}$:

$$\sigma(t) = [1 - D(\delta, t)]\bar{\sigma}(\delta, t) \quad (1)$$

Here, at each time t, the damage variable D is a nonlinear functional of δ, whereas $\bar{\sigma}$ is the interface stress that would be obtained, in the absence of damage, as the response of the fractional standard linear solid (FSLS) model depicted in Fig. 1 to the prescribed history δ.

In Fig. 1, E_1 and E_2 denote the stiffness values of the springs in the elastic and inelastic arms, respectively; α and $\hat{\eta}$ denote the relative displacement and material constant of the Scott Blair element, so that the stress σ_{SB} in the Scott Blair element is related to α through the fractional equation

$$\sigma_{\mathrm{SB}} = \hat{\eta}_0 D_t^{\nu} \alpha \quad (2)$$

where ${}_0D_t^{\nu}$ represents the fractional derivative operator of order ν, with $0 < \nu < 1$.

Setting $\hat{\lambda} = \hat{\eta}/E_2$ and $\hat{\gamma} = \hat{\lambda}(E_1 + E_2)$, $\bar{\sigma}$ is the solution to the following fractional differential equation governing the FSLS model:

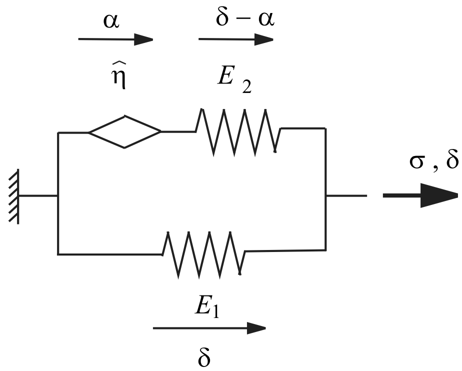

Fig. 1. Rheological representation of cohesive zone specialization of the FSLS model

$$\bar{\sigma} + \hat{\lambda}_0 D_t^\nu \bar{\sigma} = E_1 \delta + \hat{\gamma}_0 D_t^\nu \delta \quad (3)$$

Numerically, the solution of Eq. (3) is determined, in this paper and Musto and Alfano (2015), via the Grünwald-Letnikov expression of the fractional derivative (Grünwald 1867; Schmidt and Gaul 2002; Padovan 1987), by sampling the histories of δ and $\bar{\sigma}$ backward at time intervals Δt_{GL}, so that the following approximation of the fractional derivatives is obtained (Musto and Alfano 2015):

$$_0D_t^\nu \bar{\sigma} \cong \Delta t_{\mathrm{GL}}^{-\nu}[\bar{\sigma}(t) + S_\sigma] \qquad _0D_t^\nu \delta \cong \Delta t_{\mathrm{GL}}^{-\nu}[\delta(t) + S_\delta] \quad (4)$$

where

$$S_\sigma = \sum_{j=1}^{N_h-1} A_{j+1} \bar{\sigma}(t - j\Delta t_{\mathrm{GL}}) \qquad S_\delta = \sum_{j=1}^{N_h-1} A_{j+1} \delta(t - j\Delta t_{\mathrm{GL}}) \quad (5)$$

A_{j+1}, are the Grünwald-Letnikov coefficients, which are given by the following recursive formula:

$$A_{j+1} = \frac{\Gamma(j-\nu)}{\Gamma(-\nu)\Gamma(j+1)} = \left(\frac{j-1-\nu}{j}\right)\frac{\Gamma(j-1-\nu)}{\Gamma(-\nu)\Gamma(j)} = \frac{j-1-\nu}{j} A_j, A_1 = 1 \quad (6)$$

where Γ = gamma function.

In this way, the numerical solution of Eq. (3) is given by

$$\bar{\sigma}(\delta, t) = (1 + \hat{\lambda}\Delta t_{\mathrm{GL}}^{-\nu})^{-1}[(E_1 + \hat{\gamma}\Delta t_{\mathrm{GL}}^{-\nu})\delta(t) + \Delta t_{\mathrm{GL}}^{-\nu}(\hat{\gamma} S_\delta - \hat{\lambda} S_\sigma)] \quad (7)$$

Thermodynamic Formulation and Damage Evolution Law

Eqs. (1) and (3) can be considered a special case of a more general model in which damage is coupled with linear viscoelasticity, which can be rewritten in integral form as follows:

$$\sigma(t) = (1 - D(t)) \int_0^t G(t-\tau)\dot{\delta}(\tau) d\tau \quad (8)$$

where G represents the suitable relaxation function, which does not necessarily have to be defined in terms of internal variables. The specialization of this general formulation, presented in this section, to the model of the previous section is provided in the Appendix for the benefit of the reader.

In the isothermal setting, the second law of thermodynamics can be expressed by introducing the free energy Ψ as follows:

$$\sigma\dot{\delta} - \dot{\Psi} \geq 0 \quad (9)$$

Following, for example, the quadratic free energy expression proposed by Breuer and Onat (1964), the assumption is made that the free energy can be described with the functional

$$\Psi(t) = [1 - D(t)] \int_0^t \int_0^t K(t-\tau_1, t-\tau_2)\dot{\delta}(\tau_1)\dot{\delta}(\tau_2) d\tau_1 d\tau_2 \quad (10)$$

where K represents the continuous, symmetric, and sufficiently smooth kernel.

Considering other possible free energy expressions (Fabrizio and Golden 2003; Amendola et al. 2014) does not alter the nature of the discussion. Differentiating Eq. (10) and inserting into Eq. (9), the following relationship is obtained:

$$\left\{\sigma(t) - [1 - D(t)]2\int_0^t K(0, t-\tau)\dot{\delta}(\tau)d\tau\right\}\dot{\delta}(t) + [1 - D(t)]\int_0^t\int_0^t\left(-\frac{\partial K}{\partial t}\right)\dot{\delta}(\tau_1)\dot{\delta}(\tau_2)d\tau_1 d\tau_2 + \dot{D}(t)\int_0^t\int_0^t K(t-\tau_1, t-\tau_2)\dot{\delta}(\tau_1)\dot{\delta}(\tau_2)d\tau_1 d\tau_2 \geq 0 \quad (11)$$

Following the Coleman-Noll procedure, given the lack of constraint on the sign of $\dot{\delta}$, yields

$$\sigma = [1 - D(t)]2\int_0^t K(0, t-\tau)\dot{\delta}(\tau)d\tau \quad (12)$$

Comparing with Eq. (8), one has

$$\int_0^t G(t-\tau)\dot{\delta}(\tau)d\tau = 2\int_0^t K(0, t-\tau)\dot{\delta}(\tau)d\tau \quad (13)$$

which represents a further restriction for K but not sufficient to determine it uniquely (Breuer and Onat 1964).

The first term in Eq. (11) being zero, it can then be appreciated that a possible choice of sufficient conditions for the validity of the inequality, for an arbitrary relative-displacement history, is that $\dot{D}$ be positive (damage irreversibility) and that

$$\int_0^t\int_0^t\left(-\frac{\partial K}{\partial t}\right)\dot{\delta}(\tau_1)\dot{\delta}(\tau_2)d\tau_1 d\tau_2 \geq 0 \quad (14)$$

which is also valid for the case without damage.

A number of possible choices that can be made for the damage evolution law in the CZM will now be considered. First, the problem will be discussed from a physical and micromechanical point of view; then a simplified analysis is presented to show that a nonmonotonic $G_c - \dot{a}$ is expected if damage is driven by the whole energy; finally the related equations describing damage evolution are presented and each of the three considered damage evolution laws is analytically studied.

Damage Evolution: Micromechanical Standpoint

For an elastomeric material, such as the one considered in Musto and Alfano (2013, 2015), it seems necessary to consider the elastic energy in the elastic arm only as the damage driver. This conclusion is based on considering the microscopic properties of elastomers. In the absence of cross-linking, “green” rubber does not display a positive long-term relaxation modulus. It is then natural to identify the elastic arm in the proposed rheology as representative of the cross links (and possibly the elastic polymer/filler interaction for a filled compound). Instead, the elastic energy stored in the inelastic arm of the FSLS model is more appropriately considered as related to the entropic elasticity characteristic of elastomeric materials. For this reason, it does not seem directly relevant to the fracturing process.

In polymers used below the glass-transition temperature, the elastic energy is primarily stored in the van der Waals interaction between neighboring chains. Indeed, the covalent links along the polymeric chain are not only stronger but loaded to their maximum capacity in a rather small quantity [Berger et al. (2003) estimate only 5% of chains are fully loaded even in a highly crystalline ultra-high-molecular-weight polyethylene (UHMWPE)]. The presence of crystalline and amorphous regions (Kausch 2005) may add complexity to the picture and is not relevant to the qualitative discussion presented here, although it could well be if a more accurate and detailed micromechanical description were to be attempted. For these reasons, it seems plausible to consider all the elastic energy as a driver to damage. It is acknowledged that, even for glassy polymers, there will still be an entropic contribution (first associated with plastic hardening by Haward 1993), but its magnitude is certainly far less than in elastomeric materials.

It is recognized that the presented picture is at this stage more heuristic than quantitative and does not take into account the important role of viscoplasticity; however, for what will be shown in this section and in the next one, it seems in agreement with experimental evidence of nonmonotonic behavior of fracture energy versus applied rate in some glassy polymer resins, as noted, for example, by Frassine et al. (1993, 1995).

Nonmonotonicity of Fracture Energy with Crack Speed

For simplicity, the CZM proposed in Musto and Alfano (2013) is considered. This CZM can be schematized with a SLS model whose response is scaled by a factor $1 - D$ to account for damage and to investigate different options for the damage evolution law in addition to what is considered in Musto and Alfano (2013). However, the considerations made here will be more general and will help explicate the analysis later in the paper and the numerical results presented for the fractional CZM presented in Musto and Alfano (2015), but again considering a wider range of damage evolution laws.

If it is assumed that failure occurs suddenly (i.e., D instantaneously increases from 0 to 1) when the elastic arm reaches a predefined energy level, the fracture criterion turns out to be displacement based. The macroscopic fracture energy is then given by the elastic energy in the elastic arm plus the work done on the inelastic arm until the (fixed) failure total relative displacement. The fracture energy is therefore the sum of the elastic energy in the springs at the moment of failure plus the energy dissipated in the dashpot because of viscosity, and it turns out to be increasing for an increasing rate of applied displacement. In the slow limit, the spring in the Maxwell arm is completely relaxed such that no energy is spent there, and the viscous dissipation in the dashpot is zero so that the fracture energy attains its minimum value. In the fast limit, the dashpot does not have time to undergo any displacement, so the viscous dissipation is zero again; however, the spring is fully elongated and therefore the maximum elastic energy is spent in the Maxwell arm and the overall fracture energy attains its maximum value.

If all the elastic energy is chosen to drive damage, then interesting behavior arises. First, it is worth recalling that, for the case under examination, “all the elastic energy” means the sum of the energies in the two springs of the elastic and inelastic (Maxwell) arms. For isothermal processes and in the absence of damage, this would be equal to the specific free energy at the interface point, whose definition is unique in this case (Graffi and Fabrizio 1989).

To investigate this case, for illustration purposes a constant relative displacement rate $\dot{\delta} = \upsilon$ is considered. Again, it is assumed that failure occurs suddenly when the sum of the elastic energies in the elastic arm and the Maxwell arm reaches a threshold energy. The fracture energy G_c equals the work W_f done by the stress up to failure and, as a function of the constant applied relative displacement rate υ, is given by

$$G_c = W_f = \int_0^{t_f} \sigma(\tau)\upsilon d\tau \tag{15}$$

where t_f represents the time at which failure occurs, itself a function of the rate υ.

It is argued that G_c is not necessarily monotonic with υ. Indeed, there could exist a rate $\bar{\upsilon}$ for which G_c is maximum.

To see this, the energy $\mathcal{D}$ dissipated in the Maxwell arm up to a point in time t is considered. This is given by the work done on the element minus the stored energy in the elastic Maxwell spring, and is nonmonotonic: it is continuous and tends to zero for vanishingly slow and fast applied υ (up to a fixed relative displacement). Because it is also required to be non-negative at all times, it displays a maximum, say for $\upsilon = \bar{\upsilon}$.

If it is now assumed that the strain rate $\bar{\upsilon}$ is applied, failure will occur at time $\bar{t}_f$.

The macroscopic fracture energy will be given by

$$\bar{G}_c = \bar{\mathcal{E}}_{1f} + \bar{\mathcal{E}}_{2f} + \bar{\mathcal{D}}_f \tag{16}$$

where $\bar{\mathcal{E}}_{1f}$ and $\bar{\mathcal{E}}_{2f}$ = energies in the elastic and Maxwell arms, respectively, at $\bar{t}_f$; and $\bar{\mathcal{D}}_f$ = energy dissipated in the Maxwell arm between times 0 and $\bar{t}_f$.

If the applied rate υ is now infinitesimally varied, failure will occur at times t_+ and t_- for increased and decreased applied rate, respectively.

The fracture energy will vary of an amount dG_c:

$$dG_c = d\mathcal{E}_{1f} + d\mathcal{E}_{2f} + d\mathcal{D}_f \tag{17}$$

but

$$d\mathcal{E}_{1f} + d\mathcal{E}_{2f} = 0 \tag{18}$$

as required by the fracture criterion and $d\mathcal{D}_f = 0$ by the choice of taking $\upsilon = \bar{\upsilon}$. Because $\mathcal{D}_f$ is a maximum, this proves that G_c attains a maximum, too, at $\bar{t}_f$.

Remark 1. Other physical mechanisms and models capable of reproducing nonmonotonicity of the $G_c - \upsilon$ (or, equivalently, $G_c - \dot{a}$) relationship do exist; a review is given in Musto (2014). To the best of the authors' knowledge, though, current explanations are of a structural nature. For example, the celebrated “viscoelastic trumpet” model by De Gennes (1997) explains the decrease in fracture energy on reaching a crack speed threshold by invoking the finiteness of the test specimen. Explanations based on crack-tip branching (Kinloch and Young 1983) or periodic interface void formation (Musto 2014) are based on structural features as well. On the other hand, the model presented herein is fully local and able to exhibit nonmonotonicity even for a single material point.

Such behavior is very interesting in that the descending branch of the $G_c - \upsilon$ function can be associated with instabilities, such as stick-slip behavior (Maugin 1999; Kumar and Ananthakrishna 2010; Ciccotti et al. 2004; Kovalchick et al. 2014).

Damage Evolution Laws

In this section, the damage evolution law for the fractional CZM proposed in Musto and Alfano (2015) will be revisited and modified to allow the possibility of letting damage be driven not only by the energy in the elastic arm but also by some of, or the whole, remaining part of the free energy. To this end, the following (specific) energy variable Y is introduced:

$$Y = Y_1 + aY_2 + bY_{\rm SB} \tag{19}$$

where two parameters a and b are discussed below; Y_1 and Y_2 represents the elastic energies in the springs of the elastic and inelastic arms, respectively, for the undamaged material, given by

$$Y_1 = \frac{1}{2}E_1\delta^2 \qquad Y_2 = \frac{1}{2}E_2(\delta - \alpha)^2 \tag{20}$$

and $Y_{\rm SB}$ represents the free energy in the Scott Blair element. For this one a choice needs to be made, and the following general expression of the free energy, derived from Staverman and Schwarzl (1952), Bland (1960), and Hunter (1961) and specialized to the Scott Blair element, is considered:

$$Y_{\rm SB}(t) = \frac{\hat{\eta}}{2\Gamma(1-\nu)}\int_0^t\int_0^t (2t - \tau_1 - \tau_2)^{-\nu}\dot{\alpha}(\tau_1)\dot{\alpha}(\tau_2)d\tau_1 d\tau_2 \tag{21}$$

As discussed in the "Introduction," this choice can be physically justified by considering for the Scott Blair element the mechanical analogue proposed in Di Paola and Zingales (2012) and Deseri et al. (2014).

The double integral in Eq. (21) is evaluated numerically by dividing the interval $[0, t]$ into a number N of sufficiently refined subintervals $[t_i, t_{i+1}]$, for each of them considering the midpoint τ_i and evaluating both $2t - \tau_1 - \tau_2$ and $\dot{\alpha}$ at τ_i and τ_j, for $i, j = 1, \ldots, N$. Furthermore, $\dot{\alpha}$ is calculated as the midpoint finite difference.

The two parameters a and b can range between 0 and 1, and three possible cases will be considered:

- $a = b = 0$: in this case, damage is driven only by the energy in the elastic arm of the FSLS model, as in Musto and Alfano (2015);
- $a = 1$; $b = 0$: in this case, damage is driven by the energies in the two springs of the elastic and inelastic arms; and
- $a = b = 1$: in this case, damage is driven by the entire free energy (i.e., including the energy stored in the Scott Blair element of the FSLS model).

The damage evolution law is then written as follows:

$$\dot{D} \geq 0 \qquad Y - Y_c \leq 0 \qquad (Y - Y_c)\dot{D} = 0 \tag{22}$$

where Y_c represents an energy threshold value. If Y_c is kept fixed, sudden failure occurs because, as soon as $Y = Y_c$, $\dot{D}$ can attain any positive value, which normally results in D increasing instantaneously from 0 to 1. This brittle response would be difficult to handle computationally and would not be realistic for quasi-brittle or ductile material interfaces. This is why in CZMs a regularized law is typically used, whereby Y_c is taken as a function of D. Here the same type of regularization is used as in Musto and Alfano (2015), given by

$$Y_c = \frac{G_0}{(1 - \beta D)^2} \tag{23}$$

In the rate-independent case (or here in the slow and fast limit), this expression results in the widely used bilinear traction-separation law (Musto and Alfano 2015). The initial energy threshold G_0 is the "initiation" value that the energy needs to reach before decohesion starts.

Remark 2. It is important to underline that, in general, Y is not equal to the partial derivative of the free energy with respect to D, except for the case $a = b = 1$, as discussed in the Appendix. Indeed, it is often assumed that the damage-driving energy is the partial derivative of the free energy with respect to damage, but it is not necessary for thermodynamic consistency, for which it is sufficient to have $\dot{D} \geq 0$, as already observed.

Further Analysis of the Three Possible Damage Evolution Laws

The choice of free energy in the Scott Blair element is equivalent to specializing the general form of the free energy considered in Eq. (10) to the following:

$$\Psi(t) = [1 - D(t)][(Y_1(t) + Y_2(t) + Y_{\rm SB}(t)] \tag{24}$$

The "rupture dissipation" Π_r, which is the energy lost per unit of time as a result of decohesion but not including the viscous dissipation, is given by the third term of Eq. (11) in the general case, which here specializes to

$$\Pi_r(t) = [Y_1(t) + Y_2(t) + Y_{\rm SB}(t)]\dot{D}(t) \tag{25}$$

The total "rupture energy" dissipated is given by

$$\int_0^{+\infty} \Pi_r dt \tag{26}$$

Damage Driven by the Entire Free Energy

From Eq. (22) one has that $\dot{D}$ is always non-negative and, when $\dot{D} > 0$, it must be $Y = Y_c$. If $a = b = 1$ in Eq. (19) (i.e., if damage is driven by the entire free energy), the result is

$$Y_1(t) + Y_2(t) + Y_{\rm SB}(t) = Y(t) \tag{27}$$

and therefore

$$\int_0^{+\infty} \Pi_r dt = \int_0^{+\infty} Y(t)\dot{D}(t)dt = \int_0^1 Y_c(D)dD = \int_0^1 \frac{G_0}{(1-\beta D)^2}dD = \frac{G_0}{1-\beta} = G_{cr} \tag{28}$$

In other words, if damage is driven by the whole free energy, the energy dissipated because of decohesion is always the same and equal to $G_{cr} = G_0/(1 - \beta)$. The three values G_{cr}, G_0, and β are model input parameters, but only two of them are independent; the other is obviously obtainable from the other two.

The rest of the energy dissipated is due to viscous dissipation and can be indicated by G_{cv}. In the general case, from Eq. (11) the result is

$$G_{cv} = \int_0^{+\infty}\left\{[1 - D(t)]\int_0^t\int_0^t\left(-\frac{\partial K}{\partial t}\right)\dot{\delta}(\tau_1)\dot{\delta}(\tau_2)d\tau_1 d\tau_2\right\}dt \tag{29}$$

The whole measured fracture energy, G_c, which is the total energy dissipated per unit of cracked surface, is the sum of G_{cr} and G_{cv}:

$$G_c = G_{cr} + G_{cv} \quad (30)$$

The first term is constant, whereas G_{cv} is always positive and tending to zero in the slow and fast limits. Therefore, when the whole energy is used to drive damage, it is expected that the $G_c - \dot{\delta}$ curve (analogous to the fracture energy with regard to crack speed, $G_c - \dot{a}$, normally considered in fracture mechanics) has a bell shape, which is a result analogous to the one obtained earlier for a simplified analysis of a nonregularized damage evolution law.

Damage Driven by the Energy in the Two Springs of the FSLS Model

If damage is driven by the energy in the two springs of the FSLS model, but not by the energy in the Scott Blair element, then $a = 1$ and $b = 0$ in Eq. (19), so that one has

$$Y(t) = Y_1(t) + Y_2(t) \quad (31)$$

Therefore, in this case Eq. (28) becomes

$$\begin{aligned}\int_0^{+\infty} \Pi_r dt &= \int_0^{+\infty} [Y_1(t) + Y_2(t) + Y_{\mathrm{SB}}(t)]\dot{D}(t)dt \\ &= \int_0^{+\infty} [Y_1(t) + Y_2(t)]\dot{D}(t)dt + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt \\ &= \int_0^{+\infty} Y(t)\dot{D}(t)dt + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt \\ &= G_{cr} + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt \end{aligned} \quad (32)$$

and the total energy dissipated per unit of cracked surface is given by

$$G_c = G_{cr} + G_{cv} + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt \quad (33)$$

Although here G_{cv} has the same expression as in Eq. (29), because of different damage evolution the values are normally not the same. Nevertheless, they are expected to be of a similar order of magnitude. Hence, the presence of the third non-negative term in Eq. (35) means that the total fracture energy is larger than in the previous case, where damage is driven by the whole free energy. On the other hand, the additional third term tends to zero in the slow and fast limit such that the $G_c - \dot{\delta}$ curve is expected to have a bell shape in this case, too.

Damage Driven by the Energy in the Elastic Arm Only

If damage is driven by the energy in the elastic arm only, then $a = b = 0$ and $Y(t) = Y_1(t)$, so that

$$\begin{aligned}\int_0^{+\infty} \Pi_r dt &= \int_0^{+\infty} Y_1(t)\dot{D}(t)dt + \int_0^{+\infty} [Y_{\mathrm{SB}}(t) + Y_2(t)]\dot{D}(t)dt \\ &= G_{cr} + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt + \int_0^{+\infty} Y_2(t)\dot{D}(t)dt \end{aligned} \quad (34)$$

and the total energy dissipated per unit of cracked surface is given by

$$G_c = G_{cr} + G_{cv} + \int_0^{+\infty} Y_{\mathrm{SB}}(t)\dot{D}(t)dt + \int_0^{+\infty} Y_2(t)\dot{D}(t)dt \quad (35)$$

The fourth term represents the energy dissipated in the spring of the inelastic arm, which is therefore added to the total fracture energy (and not embedded in G_{cr}). Not only is this term expected to further raise the $G_c - \dot{\delta}$ curve, but, unlike the second and third terms, it increases with the applied speed, tending to a maximum in the fast limit; therefore, it is expected to result in a qualitative change in the curve from a bell shape to a sigmoidal shape.

Remark 3. It is worth underlining that, regardless of the choice of damage-driving energy, in the proposed model the damage evolution law [Eq. (22)] is written in a rate-independent form because the damage increase is driven by the current value only of the available energy; also, the energy threshold Y_c is a function of the current value of damage D, but does not depend on its rate or its history. This is a deliberate choice that is related to the other choice of considering damage and viscous deformation as two conceptually independent phenomena (even if they interact because they may occur at the same time), whereby damage and viscous dissipations are provided separately by the second and third term of Eq. (11). In other words, although the damage evolution is rate independent, the rate dependence of the whole interface response is the result of the rate dependence of the viscous deformation.

A possible different choice could have been to assume that the current damage evolution is also a function of the damage history. However, contrary to the presented model, in which damage is only driven by energy, assuming damage evolution to be a function of its history would be equivalent to assuming that the effective fraction of the interface on which the 'undamaged' viscoelastic behaviour applies (see also Alfano and Sacco 2006 for the concepts of 'damaged' and 'undamaged' part of an infinitesimal interface area) also plays a direct role in determining its evolution.

On the other hand, although assuming that damage evolution is function of damage history might seem appealing with a view to modeling the commonly assumed "nonlinear viscoelastic" behavior next to the crack tip, the excellent match between experimental and numerical results found in Musto and Alfano (2015) might question the need to do so.

Numerical Results and Discussion

In this section, numerical results will be presented for the pointwise interface response to a prescribed (opening) relative displacement δ at constant rate $\dot{\delta} = v$. Two cases are studied. The first is the rubber interface within the double cantilever beam (DCB) considered in Musto and Alfano (2015), in which all interface parameters are the same as in Musto and Alfano (2015) and, in particular, the fractional exponent used is 0.23. For this reason, it will be denoted "elastoviscous" case (Di Paola and Zingales 2012; Deseri et al. 2014).

In the second case, the same values for G_{cr}, G_0, E_1, and E_2 are taken but ν and $\hat{\lambda}$ are changed. The aim is to consider a "viscoelastic" case symmetric to the first "elastoviscous" case with respect to the value $\nu = 0.5$ that separates elastoviscous from viscoelastic behavior according to the definitions in Di Paola and Zingales (2012) and Deseri et al. (2014). Therefore, for this second case the fractional exponent ν is taken equal to 0.77. In order to have the same (fractional) relaxation time, which can be taken equal to $\hat{\lambda}^{1/\nu}$ and for the first case is equal to 37.39 s, the value $\hat{\lambda} = 37.39^{0.77} = 16.256\mathrm{s}^{\nu}$ is chosen. The input parameters are summarized in Tables 1 and 2.

Fig. 2 shows the traction-separation curves obtained in the elastoviscous case by considering the three damage evolution laws obtained by choosing $a = b = 0$ in Eq. (19) for a first set of simulations, $a = 1$ and $b = 0$ for a second set, and, finally $a = b = 1$ for a third set. In each simulation, the relative displacement is prescribed, at constant speed, with constant increments that in most

Table 1. Input Parameters Used in Both Cases

Parameter	Value
G_{cr} (N mm^{-1})	1.50
G_0 (N mm^{-1})	0.6
E_1 (MPa)	0.469
E_2 (MPa)	9.09

Table 2. Input Parameters Used in Each of the Two Cases

Parameter	Value
Elastoviscous case	
$\hat{\lambda}$ (s$^{\nu}$)	2.3
ν	0.23
Viscoelastic case	
$\hat{\lambda}$ (s$^{\nu}$)	16.256
ν	0.77

cases are 0.1 mm. In few cases, it can be seen in Figs. 2(b and c) that at fast rates the "failure" relative displacement reduces to values lower than 1 mm. For these cases, in order to increase the accuracy of the results and in particular the accuracy of the computation of G_c (equal to the area under the curve), the prescribed incremental displacement has been reduced to 0.025 mm. In addition to this precaution, the accuracy of the analysis has been checked and the time increments in Eq. (7) and those for the numerical integration of Eq. (21) are small enough so that their further reduction would lead to negligible changes that could not be visually appreciated in the plots.

Fig. 3 shows the fracture energy G_c against the prescribed relative-displacement speed v for the elastoviscous case [Fig. 3(a)] and for the viscoelastic case [Fig. 3(b)]. The first observation that can be made is that the results are in agreement with the analyses made earlier in this paper. In particular, when damage is driven only by the energy in the elastic arm, the fracture energy monotonically increases with applied speed. In contrast, when damage is driven either by the energy in both springs or, indeed, by the entire free energy, including the energy stored in the Scott Blair element, the curve is nonmonotonic, has a maximum, and in the fast and slow limits tends to the same value G_{cr}. This can be better seen in Fig. 4, where the curves for the case $a = b = 0$ have been eliminated to better appreciate the other ones.

A second interesting observation is that, when damage is driven only by the energy in the elastic arm, the fracture energy in the fast limit reaches values that are approximately 20 times higher than those in the slow limit, which could also be observed in Musto and Alfano (2015). In contrast, because of the very different behavior in the other two cases, G_c does not increase more than approximately 3 times the slow-limit value G_{cr} before decreasing to G_{cr} in the fast limit.

The input parameters are meaningful for the elastoviscous case and $a = b = 0$ because in this case the model captures the experimental results reported in Musto and Alfano (2015) with very good agreement. In all other cases, the analysis presented in this paper is only qualitative. Nevertheless, the results in this section suggest that the two different assumptions, discussed earlier with some physical arguments—that the damage can be driven only by the

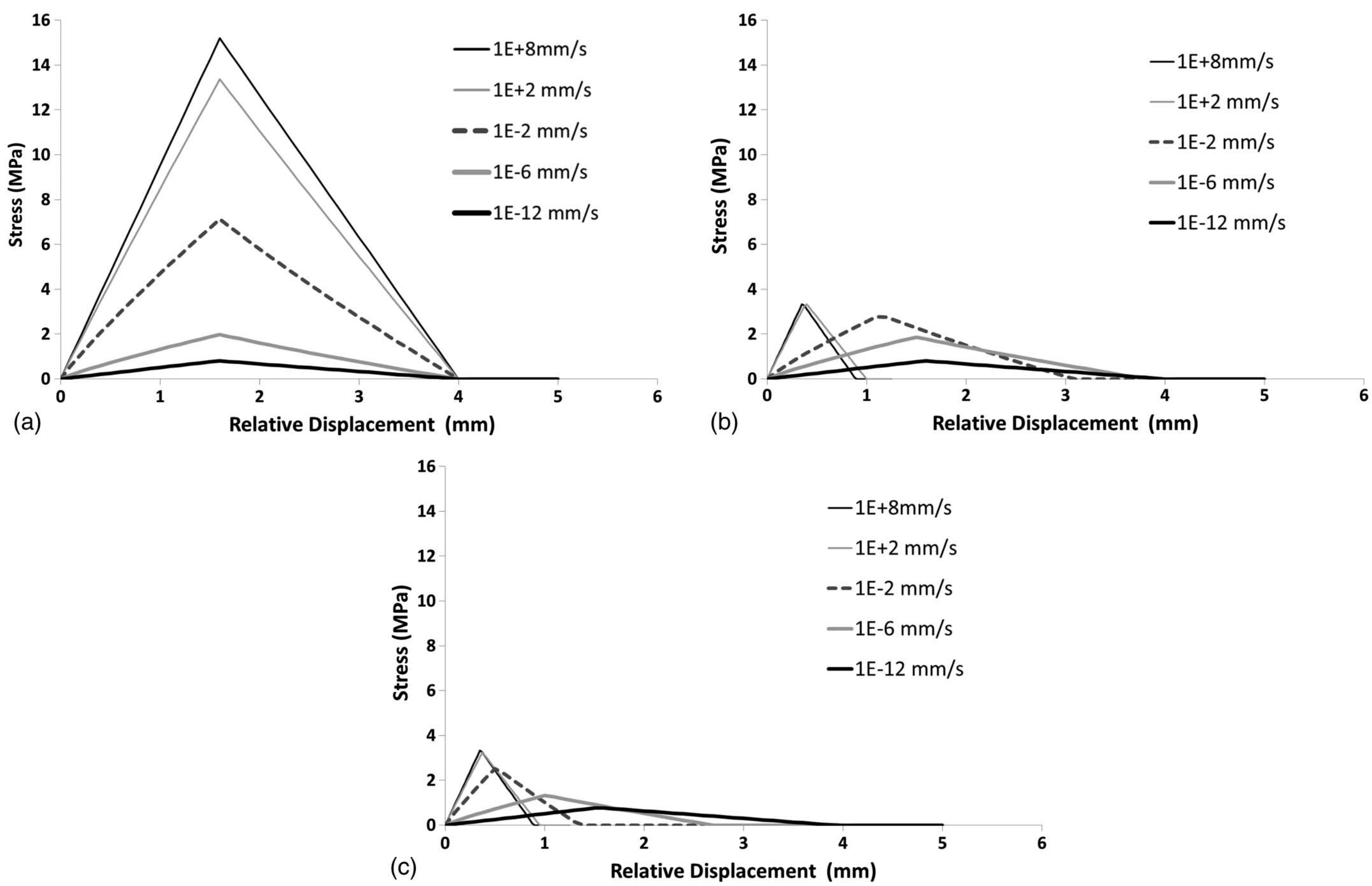

Fig. 2. Traction-separation curves for (a) $a = b = 0$; (b) $a = 1$, $b = 0$; (c) $a = b = 1$

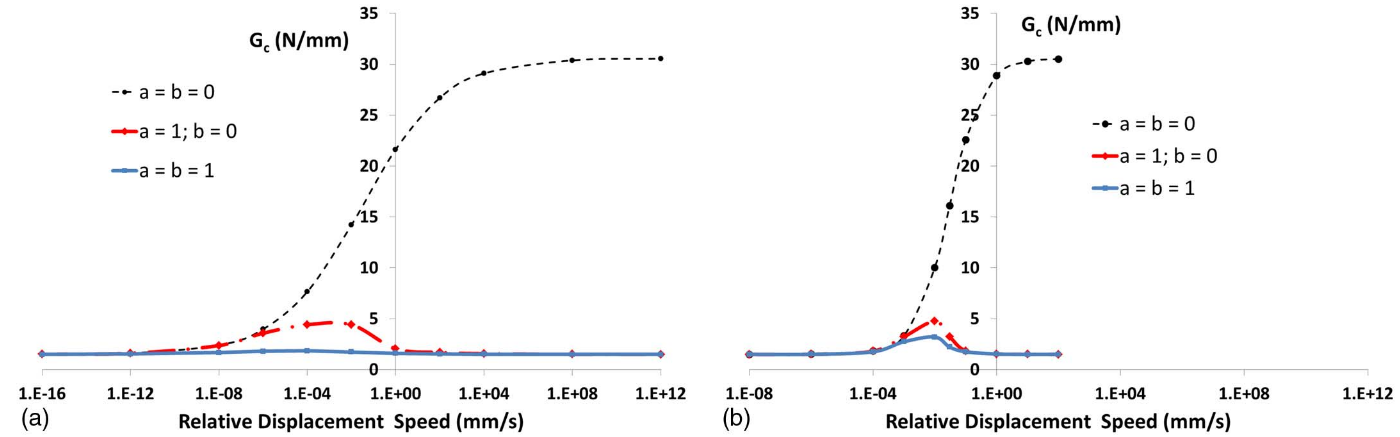

Fig. 3. Fracture energy versus applied speed for the three damage evolution laws considered: (a) elastoviscous case ($\upsilon = 0.23$); (b) viscoelastic case ($\upsilon = 0.77$)

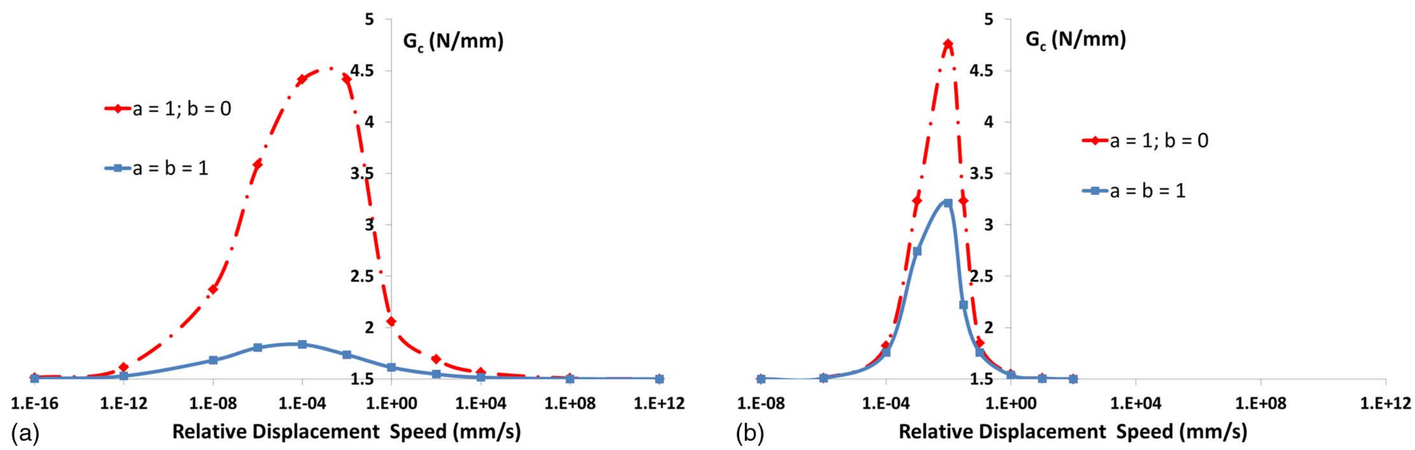

Fig. 4. Enlarged curves showing fracture energy against applied speed: (a) elastoviscous case ($\upsilon = 0.23$); (b) viscoelastic case ($\upsilon = 0.77$)

energy in the cross links or by the energy in all of the polymer chains—could potentially explain the significant difference in the rate dependence of the fracture energy experimentally observed in elastomers or glassy polymers.

When a fractional model is used, the additional question that arises is whether the free energy in Scott Blair elements can contribute to damage evolution. This is not obvious because, unlike the energy in the spring of the inelastic arm, the elastic energy stored in a Scott Blair element cannot be released instantaneously. At high speeds, the energy stored tends to zero, together with the viscous energy dissipated, but at intermediate speeds it is difficult to argue whether or not the energy stored in the Scott Blair element can be released quickly enough to be available for damage evolution. The answer to such a question will probably only come by linking the modeling approach proposed here with a detailed micromechanical analysis using an appropriate multiscale scheme to bridge the scales.

The different results for the elastoviscous and viscoelastic cases are as expected. Because in the elastoviscous case more elastic energy is stored in the elastic arm, the peak of the $G_c - \upsilon$ curve is extremely reduced and there is a more marked difference with the case where $a = 1$; $b = 0$. For the viscoelastic case, the difference is greatly reduced because of the increased amount of elastic energy stored in the Scott Blair element. This suggests that the issue of whether the energy in the Scott Blair element can or cannot contribute to damage evolution is, as expected, more important for the elastoviscous case.

Conclusions

In this paper, the fractional rate-dependent CZM proposed by Musto and Alfano (2015) has been revisited. A thermodynamic derivation has been presented, first in a form that can be applicable to a more general case in which a linear viscoelastic model is combined with damage. To specialize the formulation to the fractional model, a choice has been made regarding the free energy in the Scott Blair element of FSLS model, based on a general expression widely used in linear viscoelasticity (Staverman and Schwarzl 1952; Bland 1960; Hunter 1961), which has been shown to be valid for a mechanical analogue of a Scott Blair element (Di Paola and Zingales 2012; Deseri et al. 2014).

The novel thermodynamic derivation of the model provides a clearer framework to address and revisit the fundamental assumptions made regarding the damage evolution law. In Musto and Alfano (2015), similarly to the work by Musto and Alfano (2013) for a rate-dependent CZM building on a baseline viscoelastic model with an exponential kernel, damage is assumed to be driven by the elastic energy stored in the elastic arm of the FSLS model. This results in a relationship between total (measured) fracture energy and crack speed (or prescribed relative displacement speed) that is monotonically increasing and has a sigmoidal shape.

Here this hypothesis has been reconsidered, first by discussing the problem from a micromechanical, albeit rather qualitative, point of view. Two other possible assumptions for damage evolution have been considered. One assumes that damage is driven by the energies in the two springs of the elastic and inelastic arms; the other assumes that damage is driven by the entire free energy (i.e., including the energy stored in the Scott Blair element of the FSLS model). The three possible laws have been studied analytically and numerically, with the main finding being that, by assuming that damage is also driven by the remaining parts of the energy, a nonmonotonic relationship between total fracture energy and crack speed is obtained having a bell rather than a sigmoidal shape.

The effect of the fractional exponent ν has been shown to be significant, to the point that for low values [elastoviscous case (Di Paola and Zingales 2012; Deseri et al. 2014)] the rate dependence of the fracture energy is significantly reduced if damage is driven by the entire free energy.

The analysis presented here is mainly qualitatively, yet it suggests a physical interpretation, entirely original to the best of the authors' knowledge, for the significant differences found in the rate dependence of fracture in elastomers and glassy polymers. Although it would be misleading to draw clear conclusions from this investigation, in the authors' opinion the results presented can open very promising lines of research leading to better understanding of the rate dependence of fracture in polymeric materials. In particular, it is suggested that further studies in this direction should build on the powerful tools available in computational micro- and nanomechanics and multiscale analysis, supported by advanced micro- and nanoscale experiments.

Appendix. Thermodynamic Formulation Specialized to the FSLS Model with Damage

In this appendix, the general thermodynamic formulation presented in the paper for a general damage-viscoelastic model written using a Volterra convolution operator is specialized to the case of the model considered in the paper. In the latter, the material response is that of a FSLS model, scaled by the damage factor $1-D$.

As earlier observed, the free energy is given by Eq. (24), which is here expanded for the sake of clarity. Setting $\Psi(t)=\hat{\Psi}[\delta(t),D(t),\alpha(t),\alpha]$, one has

$$\hat{\Psi}(\delta(t),D(t),\alpha(t),\alpha)=\frac{1-D(t)}{2}\left\{E_1\delta(t)^2+E_2[\delta(t)-\alpha(t)]^2+\frac{\hat{\eta}}{\Gamma(1-\nu)}\int_0^t\int_0^t(2t-\tau_1-\tau_2)^{-\nu}\dot{\alpha}(\tau_1)\dot{\alpha}(\tau_2)d\tau_1d\tau_2\right\} \quad (36)$$

Notice that $\hat{\Psi}$ depends both on the current value of δ, D, and α at time t and on the entire history $\alpha:[0,t]\rightarrow\Re$ of the internal variable. By differentiation with respect to time, the dissipation inequality [Eq. (11)] here specializes as follows:

$$(\sigma(t)-[1-D(t)]\{E_1\delta(t)+E_2[\delta(t)-\alpha(t)]\})\dot{\delta}(t)+[1-D(t)]\left\{\frac{\hat{\eta}}{\Gamma(1-\nu)}\int_0^t(t-\tau)^{-\nu}\dot{\alpha}(\tau)d\tau-E_2[\delta(t)-\alpha(t)]\right\}\dot{\alpha}(t)$$
$$+[1-D(t)]\frac{\hat{\eta}\nu}{\Gamma(1-\nu)}\int_0^t\int_0^t(2t-\tau_1-\tau_2)^{-(1+\nu)}\dot{\alpha}(\tau_1)\dot{\alpha}(\tau_2)d\tau_1d\tau_2+\Pi_r(t)\geq 0 \quad (37)$$

where $\Pi_r(t)$ = rupture dissipation introduced in Eq. (25).

Noting that

$$E_1\delta(t)+E_2[\delta(t)-\alpha(t)]=\bar{\sigma} \quad (38)$$

where $\bar{\sigma}$ represents the interface stress in absence of damage, using standard thermodynamic arguments, Eq. (1) is obtained.

Likewise, noting that

$$\frac{1}{\Gamma(1-\nu)}\int_0^t(t-\tau)^{-\nu}\dot{\alpha}(\tau)d\tau={}_0D_t^{\nu}\alpha \quad (39)$$

and that $E_2[\delta(t)-\alpha(t)]=\sigma_{SB}$, where σ_{SB} = stress in the Scott Blair element, Eq. (2) is recovered.

The third term in Eq. (37) is the viscous dissipation (per unit of time) at time t, Π_v, which only occurs in the Scott Blair element in this case:

$$\Pi_v=[1-D(t)]\frac{\hat{\eta}\nu}{\Gamma(1-\nu)}\int_0^t\int_0^t\times(2t-\tau_1-\tau_2)^{-(1+\nu)}\dot{\alpha}(\tau_1)\dot{\alpha}(\tau_2)d\tau_1d\tau_2 \quad (40)$$

The viscous dissipation is always non-negative because the double convolution is always positive. The rupture dissipation is also always non-negative because $\dot{D}\geq 0$ in Eq. (25).

Finally, it is worth noting that the partial derivative of the free energy with respect to the damage is given by

$$\frac{\partial\hat{\Psi}}{\partial D}=\frac{1}{2}\left[E_1\delta(t)^2+E_2(\delta(t)-\alpha(t))^2+\frac{\hat{\eta}}{\Gamma(1-\nu)}\times\int_0^t\int_0^t(2t-\tau_1-\tau_2)^{-\nu}\dot{\alpha}(\tau_1)\dot{\alpha}(\tau_2)d\tau_1d\tau_2\right] \quad (41)$$

As observed earlier in the paper, although $\partial\hat{\Psi}/\partial D$ is often assumed to be the damage-driving energy in the damage evolution law, this is not necessary and only happens in the model proposed in this paper when $a=b=1$ in Eq. (19).

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