Analogies between Theories of Phase Transformations and Damage in Velcro Modelling

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Abstract. There is a deep analogy between the theory of phase transformation and various theories of damage. The analogy is reflected in the corresponding mathematical techniques – both phenomena lead to a deeply nonlinear boundary value problem with free boundaries. This principal mechanism of nonlinearity occurs even for physically and mechanically linear equations of states. It can be understood and illustrated even on the particularly simple examples relating to unzipping in Velcro systems, which are of practical interest on their own.

1. Introduction

In their early stages, theories of phase transformations and of damage/fracture were being developed independently from each other. There are various reasons for that situation. However, both disciplines have many common features that are more obvious from the microscopic than macroscopic point of view. In fact, both disciplines deal with the energy exchange between two spatial scales: between the macroscale energy, often called elastic energy, and the microscopic energy, often called the cohesion energy of the bonds. Of course, there is a lot of schematization in this counter positioning of the scales and in corresponding terminology. We refer the interested readers to the pioneering papers in both disciplines [1]-[5]. For instance, the classical paper on brittle fracture of Griffith [2] is based on the consideration of the balance between the elastic energy and surface energy. The latter of which is nothing but one the phenomenological models of the energy accumulated in the cohesion bonds. From the standpoint of the Gibbs paradigm [1] of heterogeneous systems, the analysis of Griffith is a paraphrase of analysis of the phase transformations in solids, when one of the phases is vacuum and the possible shapes of the new “phase” should be chosen among ellipsoids [6]. This analogy was developed further in the papers [8]-[12] of the US Army Research Laboratory authors, dealing with the modeling of distributed fracture based on energy minimization.

The similarity between the theories of fracture and phase transformation is somewhat less obvious on the macroscopic level than on the microscopic one. However, it does exist, and it is essential even on the level of the relevant mathematics. Namely, both phenomena lead to the partial differential equations with unknown boundaries. In other words, in both disciplines we deal with the
problems which remain essentially nonlinear even when the corresponding bulk equations are linear. In particular, the principle of superposition of solutions is not applicable to those systems.

Both problems – of phase transformations and fracture - are difficult for analytical studies. Fortunately, there is a qualitatively similar problem which is much easier to handle. It is the problem of detachment of an elastic beam from a rigid substrate introduced and analyzed by Iakov Frenkel [3] which replaces the PDE of elasticity with much simpler ODE, based on the engineering theory of beams. There is, however, even simpler model of practical importance. It is the problem of Velcro detachment. For some problems of Velcro, there is no need in using even ordinary differential equations. Instead, the problem can be reduced to minimization of algebraic function of one or two variables. Still, the model allows to penetrate deeper into the physical nature of cohesion and formal structure of more difficult mathematical problems dealing with cohesion. Below, we consider a couple of those quite elementary one-dimensional problems of Velcro. The corresponding two-dimensional problems are harder to deal with, and require more powerful techniques, described in [6]-[12].

2. A Simple Model of Velcro

State-of-the-art in modeling adhesives can be found in monographs [13]-[15]. More specific studies of Velcro are presented in reference [16]. In the 1990s, Velcro-ceramic composites were developed by the U.S. Army and U.S. Air Force for the purpose of providing armor protection. The Velcro component of the composite tiles plays two roles: (1) it provides the fastening capability and (2) it gives a degree of shock resistance essential for the survival of the brittle ceramic. An analysis of these tiles, in the current context, would require a two-dimensional (2-D) approach using partial differential equations and multi-dimensional calculus of variations. Such an analysis goes beyond the scope of this paper, which is based on one-dimensional (1-D) analysis and elementary calculus.

Consider the system shown in Figure 1. Velcro is attached to a rigid substrate.

![Figure 1. The simplest Velcro detachment experiment.](image)

The Velcro fabric is assumed to be an inextensible thread of length $L$. The thread is loaded by the weight $mg$. Let $x_f$ and $x_R$ be the coordinates of the left and right ends of the attached part of the Velcro. We assume that the Velcro has negligible resistance to bending. However, despite the fact that the Velcro is modelled to contain no (long-range) elastic energy, it nonetheless carries a (short-range) energy of distributed chemical bonds between the Velcro and its attached substrate. Let $L_{at}$ be the length of an attached part of the Velcro with the distributed chemical energy per unit length equal to $\sigma_{at}$, and $L_{dt} = L - L_{at} = L - x_R - x_f$ is the length of the detached part of the Velcro with the
distributed chemical energy per unit length equal to \( \sigma_{\text{de}} \). Then, the total accumulated chemical energy \( E_{\text{chem}} \) is given by the formula

\[
E_{\text{chem}} = \sigma_{\text{at}} L_{\text{at}} + \sigma_{\text{de}} L_{\text{de}}
\]  

(1.1)

Neglecting the radius of the pulley, we obviously have the following geometric formula for the detached part of the thread:

\[
L_{\text{de}} = h - z_w + \sqrt{h^2 + x_f^2}
\]  

(1.2)

In addition to the accumulated chemical energy equation (1.1), the system also possesses gravitational energy \( E_{\text{grav}} \). Thus, the total energy \( E_{\text{total}} \) of the system can be presented in the form

\[
E_{\text{total}} = E_{\text{grav}} + E_{\text{chem}} = mg z_w + \sigma_{\text{at}} L_{\text{at}} + \sigma_{\text{de}} L_{\text{de}}
\]  

(1.3)

or, alternatively, as

\[
E_{\text{total}} = E_{\text{grav}} + E_{\text{chem}} = mg z_w + \sigma_{\text{de}} L_{\text{de}} + \sigma_{\text{at}} \left( x_R - x_f \right).
\]  

(1.4)

In the presented model, the quantities \( \sigma_{\text{de}}, \sigma_{\text{at}}, g, x_R, L, \) and \( h \) are fixed. In essence, the total energy \( E_{\text{total}} \) can be presented as a function of a single variable \( x_f \):

\[
E_{\text{total}} = E_{\text{grav}} + E_{\text{chem}} = mg \left( \sqrt{h^2 + x_f^2} - x_f \right) + \sigma_{\text{eff}} x_f + C
\]  

(1.5)

where

\[
\sigma_{\text{eff}} = \sigma_{\text{de}} - \sigma_{\text{at}}
\]  

(1.6)

and \( X \) is a constant (see the derivation in the Appendix 1).

3. Conditions of Equilibrium of Inextensible Velcro

The condition of equilibrium of the Velcro with respect to the coordinate \( x_f \) of detachment can be found by equating to zero the first derivative of the function \( E_{\text{total}}(x_f) \):

\[
\frac{dE_{\text{total}}}{dx_f} = mg \left( \frac{x_f}{\sqrt{h^2 + x_f^2}} - 1 \right) + \sigma_{\text{eff}} = 0
\]  

(2.1)

In terms of the angle \( \theta \), shown in the figure 1, the equation (2.1) can be rewritten as follows:
We can also write equation (2.2) as follows:

\[ \sin^2 \frac{\theta}{2} = \frac{\sigma_{\text{eff}}}{2mg} \]  

(2.3)

In the system described, the loading of the Velcro was made by gravity. In this very system, however, the force \( mg \) could obviously have been replaced by an equivalent tension \( T \) applied to the Velcro. Thus, it is reasonable to rewrite equation (2.3) as

\[ \sin^2 \frac{\theta}{2} = \frac{\sigma_{\text{eff}}}{2T} \]  

(2.4)

So far, we have established formula (2.4) for the case of gravitational loading only. It is rather appealing to assume, though, that formula (2.4) has much wider applications for different loading. This is not as obvious as one might think. In fact, the concept of force, and of tension, in particular, remains quite controversial. This is especially true when electro- and magnetostatic forces are taken into account. This is also true when the influence of the chemical bonding should be taken into account. For instance, the distinctions between the surface tension and the surface energy remain an issue of intense debate. From the conceptual standpoint, it is remarkable and instructive that in our thermodynamic analysis the concept of tension within the Velcro was completely eliminated from the derivation of the key formulas (2.2) and (2.3).

The simple equation (2.4) shows that the angle \( \theta \) diminishes when the tension \( T \) grows. In particular, the angle approaches zero when the tension approaches infinity - this qualitative conclusion seems intuitively transparent. The quantitative validity of this formula requires, as always, experimental verification.

For the angle \( \theta = \pi / 2 \), the formula (2.4) implies

\[ \sigma_{\text{eff}} = mg \]  

(2.5)

Its physical meaning is absolutely transparent. At this very angle, the incremental detachment \( dx_f \), causing the release the chemical energy \( dE_{\text{chem}} = (\sigma_{\text{de}} - \sigma_{\text{at}})dx_f \), completely converts into the decrease of the load height \( -dz_f = dx_f \), causing consumption of the gravitational potential \( dE_{\text{grav}} = -mgdz_f = mgdx_f \). By equating these energy increments, we arrive at formula (2.5). It can be used, however, for the macroscopic interpretation and measurement of the microscopic (or, if one wishes, nanoscale) concept \( \sigma_{\text{eff}} \).

The magnitude of \( \sigma_{\text{eff}} = \sigma_{\text{de}} - \sigma_{\text{at}} \) can, in fact, change in time due to various micro- and nanoscale phenomena like chemical contamination, absorption, desorption, environmental changes, etc. The result will be indicated by the macroscopic variation in the detachment length.

4. Condition of Stability of Inextensible Velcro

The issue of stability of the equilibrium configuration can be addressed by calculating the second derivative of the function \( E_{\text{total}}(x_f) \). The direct calculation gives us
According to equation (3.1), the second energy variation is always greater than zero. Thus, in the framework of thermodynamic theory, the equilibrium configuration is always stable.

5. Extensible Velcro Model

We can make one more important extension to the model without any necessity for considering ordinary or partial differential equations.

We now assume that the total internal energy \( E_i \) of the system consists of the distributed “elongation” energy \( E_{el} \), accumulated in the detached part of the stretched thread, and the distributed “chemical” energy \( E_{chem} \) of the Velcro bonds:

\[
E_i = E_{el} + E_{chem}. \tag{4.1}
\]

We assume that the attached part of the Velcro cannot undergo any stretching. Let \( E_{el} \) be defined by the following relationship:

\[
E_{el} = L_{de} \epsilon(\lambda) \tag{4.2}
\]

where \( L_{de} \) is the “reference” length of the detached part of the thread and \( \lambda \) is the elastic elongation of the thread.

The total chemical energy of the system is equal to

\[
E_{chem} = \sigma_{de}(\lambda) L_{de} + \sigma_{at}(x_R - x_f) \tag{4.3}
\]

where \( \sigma_{de}(\lambda) \) is a positive material function and \( \sigma_{at} \) is a positive material constant.

In this case, the total energy \( E_{total}^{ext}(x_f, \lambda) \) is given by an expression analogous to equation (1.5):

\[
E_{total}^{ext}(x_f, \lambda) = mg \left[ \sqrt{h^2 + x_f^2} + (x_R - x_f - L^*) \lambda \right] -
\left[ \sigma_{de}(\lambda) + e(\lambda) \right] (x_R - x_f - L^*) - \sigma_{at} x_f + C^* \tag{4.4}
\]

where \( L^* \) is the Velcro’s full unscratched “reference” length and

\[
C^* \equiv \sigma_{at} x_R + mgh. \tag{4.5}
\]

In the case when the surface energy \( \sigma_{de} \) of the detached film is independent of \( \lambda \), the equations (4.4), (4.5) can be replaced with the following expression:
6. Conditions of Equilibrium of Extensible Velcro

Equating to zero the first derivative of the energy \( E_{\text{total}}^{\text{ext}}(x_f, \lambda) \), we arrive at the following equations of equilibrium:

\[
\frac{\partial E_{\text{total}}^{\text{ext}}(x_f, \lambda)}{\partial \lambda} = mg\left(x_R - x_f - L\right) - \left(\frac{d\sigma_{de}}{d\lambda} + \frac{de}{d\lambda}\right)x_f = 0
\]

(5.1)

and

\[
\frac{\partial E_{\text{total}}^{\text{ext}}(x_f, \lambda)}{\partial x_f} = mg\left(\frac{x_f}{\sqrt{h^2 + x_f^2}} - \lambda\right) + \sigma_{de} - \sigma_{aw} + e = 0
\]

(5.2)

The force equilibrium condition (5.1) implies the relationship

\[
\frac{de}{d\lambda} = mg - \frac{d\sigma_{de}}{d\lambda}
\]

(5.3)

Traditionally, the derivative \( de/d\lambda \) would be identified with the tension \( T \) of the extensible thread. Formula (5.3) indeed confirms this vision, provided that the surface tension \( \sigma_{de} \) is zero or that it is independent of the elongation. However, that is not the case. There is a nontrivial dependence of \( \sigma_{de} \) on \( \lambda \). Such a dependence is not something exotic. On the contrary, it is a typical situation in physical chemistry, and in mechanochemistry, in particular.

Let us turn now to the condition of chemical equilibrium (5.2). With the help of the condition of mechanical equilibrium (5.3), we can rewrite equation (5.2) as follows:

\[
mg\left(\frac{x_f}{\sqrt{h^2 + x_f^2}} - \lambda\right) + \sigma_{de} - \sigma_{aw} + e = 0
\]

(5.4)

or alternatively as

\[
\frac{d}{d\lambda} \left(\frac{e + \sigma_{de} - \sigma_{aw}}{\lambda}\right) = 0
\]

(5.5)

Consider the model of extensible Velcro described by the following conditions:
\[ \sigma_{de} = \text{const}, \ e = \frac{1}{K}(\lambda - 1)^2. \quad (5.6) \]

In this case, the equilibrium equations (5.3), (5.4) provide the relationships

\[ K(\lambda - 1) = mg \]

and

\[ mg \left( \frac{x_f}{\sqrt{h^2 + x_f^2}} - \lambda \right) + \frac{K}{2}(\lambda - 1)^2 + \sigma_{de} - \sigma_{st} = 0. \quad (5.8) \]

With the help of equation (5.7), equation (5.8) can be rewritten as follows:

\[ \lambda - \cos \theta = \frac{mg}{2K} + \frac{\sigma_{de} - \sigma_{st}}{mg}. \quad (5.9) \]

which generalizes equation (2.2) and allows the calculation of the corrections for the finite magnitude of the elasticity modulus \( K \).

7. Condition of Stability of Extensible Velcro

Calculating the second derivative of energy in vicinity of equilibrium configuration, we get

\[
\begin{align*}
\frac{\partial^2 E^{\text{ext}}_{\text{total}}(x_f, \lambda)}{\partial \lambda^2} &= \frac{d^2(\sigma_{de} + e)}{d\lambda^2} \left( L - x_h + x_f \right) \\
\frac{\partial^2 E^{\text{ext}}_{\text{total}}(x_f, \lambda)}{\partial \lambda \partial x_f} &= 0 \\
\frac{\partial^2 E^{\text{ext}}_{\text{total}}(x_f, \lambda)}{\partial x_f^2} &= \frac{mg}{\left( h^2 + x_f^2 \right)^{3/2}}
\end{align*}
\]

In the case of constant surface energy density, equation (6.1) implies stability of the equilibrium configurations.

8. Conclusion

We formulated the simplest 1D model of a Velcro-like adhesive and applied it to an analysis of equilibrium and stability, using an energy (variational) approach. The Velcro was assumed to be partially attached to a rigid substrate. No assumption of small displacement of the Velcro was made. For the cases of inextensible and extensible Velcro, the analysis appeared to be rather elementary and required only the standard techniques of multivariate calculus. No special knowledge of differential equations was required. We established the conditions of equilibrium for the system and proved that those configurations are always stable.

The model used here is a direct analogy of the Griffith crack model of brittle fracture. In the Griffith approach, the energy of the bond is modeled by introducing a constant called surface tension. The Griffith model was justly criticized by Iakov Frenkel’ [10], who suggested a remedy based on introducing a finite zone of partial decohesion. This idea was further developed by many researchers,
starting with the pioneering publications of Barenblatt et al. [11]. In the zone of partial decohesion, the molecular interaction is modeled with extensible springs.

The analysis of 2D problems, including the intriguing problem of morphological stability of the decohesion curve requires much more powerful techniques presented in [6]. Such morphological instabilities if confirmed theoretically and experimentally can shed light on various conceptual paradoxes of the Gibbs paradigm discussed in [6].

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Appendix 1. Derivation of (1.5), (1.6)
With the help of the relationship (1.2) we can rewrite the total energy in the form

\[ E_{\text{total}} = m g z_w + \sigma_{kk} \left( h - z_w + \sqrt{h^2 + x_j^2} \right) + \sigma_{\alpha\tau} \left( x_k - x_j \right). \]  (7.1)
The coordinate $z_w$ can be excluded from the expression of the total energy, equation (7.1), with the help of the geometric formula for the total length:

$$h - z_w + \sqrt{h^2 + x_f^2} + x_R - x_f = L,$$  

(7.2)

implying

$$z_w = h + \sqrt{h^2 + x_f^2} + x_R - x_f - L.$$  

(7.3)

Eliminating $z_w$ between equations (7.1), (7.3), we arrive at the expression (1.5); The constants $\sigma_{eff}$ and $C$ are given by the formulas

$$\sigma_{eff} \equiv \sigma_{de} - \sigma_{at},$$

$$C \equiv mgh(h + x_R - L) + \sigma_{de}L - (\sigma_{de} - \sigma_{at})x_R.$$  

(7.4)

Appendix 2. Derivation of (4.6), (4.7)

With the help of (4.1)-(4.3), we can rewrite the total energy in the form

$$E_{total}^{ext} = mgz_w + \sigma_{de}(\lambda)\frac{1}{\lambda}(h - z_w + \sqrt{h^2 + x_f^2}) + \sigma_{at}(x_R - x_f)$$  

(7.5)

The coordinate $z_w$ can be eliminated from the expression for the total energy, equation (7.1), with the help of the geometric formula of the total length

$$\frac{1}{\lambda}(h - z_w + \sqrt{h^2 + x_f^2}) + x_R - x_f = L$$  

(7.6)

implying

$$z_w = h + \sqrt{h^2 + x_f^2} + (x_R - x_f - L)\lambda.$$  

(7.7)

Eliminating $z_w$ between (7.1) and (7.3), we arrive at the following chain of relationships:

$$E_{total}^{ext} = mgz_w + \sigma_{de}(\lambda)\frac{1}{\lambda}(h - z_w + \sqrt{h^2 + x_f^2}) + \sigma_{at}(x_R - x_f) =$$

$$\left[ mgz_w - \sigma_{de}(\lambda)\frac{1}{\lambda} \right] z_w + \sigma_{de}(\lambda)\frac{1}{\lambda}(h + \sqrt{h^2 + x_f^2}) + \sigma_{at}(x_R - x_f) =$$

$$\left[ mgz_w - \sigma_{de}(\lambda)\frac{1}{\lambda} \right] \left[ h + \sqrt{h^2 + x_f^2} + (x_R - x_f - L)\lambda \right] +$$

$$\sigma_{de}(\lambda)\frac{1}{\lambda}(h + \sqrt{h^2 + x_f^2}) + \sigma_{at}(x_R - x_f)$$  

(7.8)

After some regrouping in (7.8), we get
\[ E_{\text{total}}^{\text{ext}} = mg \left[ h + \sqrt{h^2 + x_f^2} + (x_R - x_f - L) \lambda \right] - \sigma_{de}\left( \lambda \right) \frac{1}{\lambda} \left[ h + \sqrt{h^2 + x_f^2} + (x_R - x_f - L) \lambda \right] + \]
\[ \sigma_{de}\left( \lambda \right) \frac{1}{\lambda} \left( h + \sqrt{h^2 + x_f^2} \right) + \sigma_{ur}\left( x_R - x_f \right) = mg \left[ h + \sqrt{h^2 + x_f^2} + (x_R - x_f - L) \lambda \right] - \]
\[ \sigma_{de}\left( \lambda \right) \left( x_R - x_f - L \right) - \sigma_{ur} x_f + \sigma_{ur} x_R + mgh \]

which immediately results in the equations (4.6), (4.7).