CONTEMPORARY RESEARCH IN THE MECHANICS AND
MATHEMATICS OF MATERIALS
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FRACTURE AS A PHASE TRANSITION

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ABSTRACT

We present an elementary one dimensional model of fracture in terms of nonlinear elasticity theory. This model essentially follows Ericksen's treatment of phase transition in an elastic bar: the energy, which is minimized subject to the standard constraints, is a nonconvex function of the displacement gradient. It represents a special case of the "double well" potential when one well is degenerate and appears at infinity. By examining a discrete system of interacting atoms, we suggest a way to bring "fracture energy" into the continuum picture; normalized interatomic length plays a role of a small parameter. In the zero order approximation we obtain a model of a bar that does not support tension. In the next order we recover a particular kind of a "cohesive zone" model which allows one to describe fracture as a bifurcation phenomenon.

1. INTRODUCTION

Significant progress has been made recently in our understanding of certain inelastic phenomena from the perspective of the elasticity theory. After the pioneering work of J.L. Ericksen [1] it became clear that nonlinear elasticity is of fundamental importance for the hysteretic behavior of shape memory alloys and other materials undergoing martensitic phase transformations. It was noticed that if the elastic energy density of the material is nonconvex (nonquasiconvex) then the solutions of the classical problems are not smooth; moreover, the regularized energy of the body made of such a material will typically exhibit an enormous multiplicity of wells corresponding to stable phase mixtures. The evolution of this system goes through a succession of microstructures and the real physical process is irreversible: when the well is being changed, high frequency vibrations of the crystal lattice are excited and this takes the energy away from the macroscopic (continuum) degrees of freedom and is seen at the continuum level as dissipation. Cryštal plasticity is a very similar phenomenon, except that at the "material" level the energy "wells" are much more numerous than in the case of phase transformation, they are farther away from each other and the barriers are higher.

In this note we show how fracture naturally fits the same framework. To illuminate the ideas we restrict the analysis to the one - dimension which, we believe captures the essence of the phenomenon. Our approach is based on the idea that energy is nonconvex with one nontrivial well at zero strain (undistorted configuration) and another a degenerate well at infinity (vacuum phase). Solutions of the equilibrium problem now lack both smoothness and continuity: the vacuum phase has a peculiar property of being localized on the set of zero measure. This is suggestive of the formation of plane cracks (voids or cavities in multidimensional setting). A straightforward application of Ericksen's ideas show that in equilibrium such material does not support tension. In an attempt to bring an

internal length scale (fracture energy) into the theory we turn to a similar discrete one - dimensional system of interacting atoms. The main feature of the phenomenon of crack formation in the discrete lattice, which is not captured by classical linear fracture mechanics, is its bifurcational character. By separating the micro from the macro degrees of freedom in our discrete model we obtain a continuum theory with an internal length scale, which turns out to be a particular kind of the cohesive zone model (Barenblatt [2]). The important feature of this theory is that it describes branching of the "cracked" states from the trivial ones. We then give a heuristic discussion of the homogenization limit in the case of multiple cracking. The corresponding "damage" theory contains an additional field of order parameter which measures local deviations from the Cauchy - Born Rule (see Ericksen [3]).

2. CRACKS IN THE ERICKSEN'S BAR

Following Ericksen [1], consider an elementary minimization problem for a one dimensional elastic bar of unit length in a hard device:

$$F\{u(x)\} = \int_0^1 f(w)dx \to \inf, \tag{2.1}$$

where the infimum is sought in the class of piecewise smooth functions which satisfy the following constraint

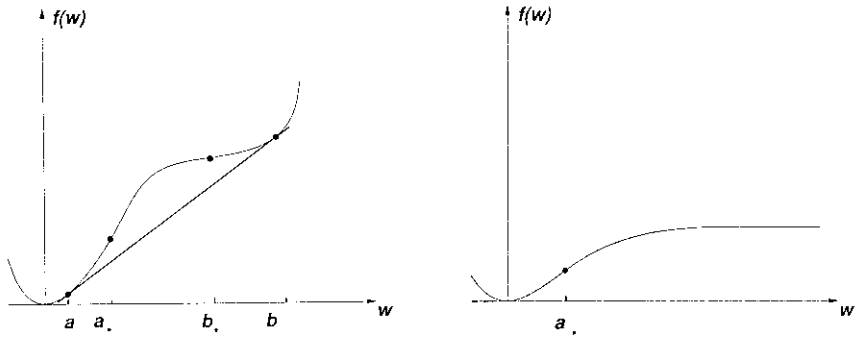
$$\int_0^1 w dx = d. \tag{2.2}$$

Here $w = u_x$ is a displacement gradient (strain), $f(w)$ is the stored energy density of the material and d is the total displacement of the bar. For the generic nonconvex energy $f(w)$ shown in Fig.1a, Ericksen found that when $a \le d \le b$ the functional (2.1) is minimized provided

$$\mathrm{w}(\mathrm{x}) = \begin{cases} a, & x \in [0,1] \setminus \Omega_b \\ b, & x \in \Omega_b \end{cases} \tag{2.3}$$

where the so-called Maxwell strains a and b are defined by the common tangent construction corresponding to the "tie-line" in Fig.1a (convexification of $f(w)$), and $meas\Omega_b = (d-a)/(b-a)$ (lever rule). This solution describes the equilibrium mixture of two phases, occupying the sets Ω_b and $[0,1] \setminus \Omega_b$.

Suppose now we fix point a and the slope of the tie-line and consider the limit $b \to \infty$; in this case a and b are maintained as the Maxwell strains. Then in Ericksen's solution $\theta = meas\Omega_b \to 0$ and $b\theta \to d-a$, which means that the measure of the set in the bar that is occupied by phase b tends to zero but the total displacement of that set is non zero. This implies that the class of functions which describe the equilibrium state of the bar in this limit must be sufficiently rough to admit displacements which have finite discontinuities on sets of zero measure. Notice also that the value of the minimum energy for the equilibrium configuration is given by $F(d) = f(a) + f'(a)(d-a)$, and is finite in the limit and independent of b.



(a) (b)

Fig. 1

The suggestion that displacement discontinuities would appear in the limit described above clearly brings to mind the idea of fracture. To pursue the analogy notice that when a bar is broken and no "surface" (or specific "fracture") energy is involved the total energy should be zero and the pieces should be unstressed. In terms of Ericksen's model this would mean that $a = 0$, $f(a) = 0$, and $f'(a) = 0$, which is not the case above. A form of the energy density $f(w)$ for which this is true is shown in Fig.1b, and is somewhat unusual since it does not satisfy the standard growth conditions necessary for the existence of the solution for a traction problem.

Notice that for this energy function the global minimum is again described by the convex envelope of the energy density $f(w)$, so a minimizing field can not support tension: for positive d the solution of (2.1 - 2.2) corresponds to unloaded segments of the bar which are separated by arbitrarily distributed cracks ($w(x)$ is a set of δ - functions). If only smooth elastic displacements $u(x)$ are allowed, the uniform (unbroken) configuration is one of minimal energy and $w(x) \equiv d$ is the strain field which minimizes the energy functional (2.1) at least for $0 \le d \le a_*$ (see Fig.1b). For $d > a_*$ a minimizer does not exist, so this constraint (smoothness) on the displacement field does not allow for the formation of cracks; in addition, it predicts an "ultimate" strength which is too high. To resolve this dilemma, we shall explore a different point of view and reexamine the phenomenon from the perspective of a crystal lattice.

3. FRACTURE IN THE SYSTEM OF FOUR ATOMS.

To obtain the simplest but still representative picture consider an ordered system of 4 interacting atoms connected by 3 nonlinear springs and having a total energy

$$V_3(r_1, r_2, r_3) = \sum_{i=1}^{3} v(r_i). \tag{3.1}$$

The atoms are constrained to lie on the straight line, r_i denotes the length of the i -th deformed spring, and $v(r)$ is the interatomic potential whose general form is shown in Fig. 2. To be definite, consider the Lennard - Jones potential

$$v(r) = A[(r_0 / r)^{12} - 2(r_0 / r)^6], \tag{3.2}$$

which is obviously a nonconvex function of r. To simplify the analysis we shall consider only the interaction between the nearest neighbors, as is clear from the form of (3.1).

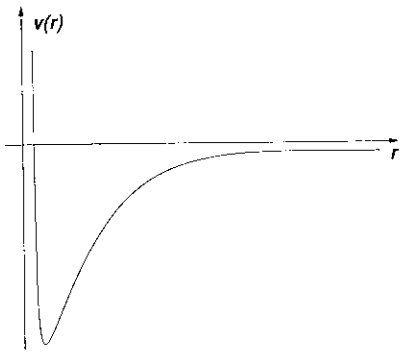


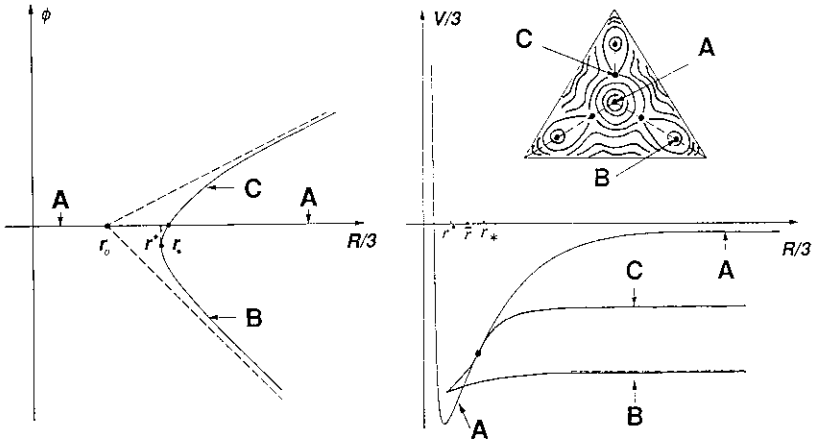
Fig. 2

Now, analogous to Sec.2, let us impose the constraint (hard device)

$$\sum_{i=1}^{3} r_i = R, \tag{3.3}$$

where $R > 0$ is given, and attempt to characterize the corresponding minimal energy configurations (i.e., the sets r_1, r_2, r_3). For the case of a "double well" energy (see Fig.1a), similar question was first addressed by Müller and Villaggio [4] in the context of plasticity theory.

The problem (3.1, 3.3) has essentially one degree of freedom, and is elementary. Clearly, if the atoms are uniformly spaced (Cauchy-Born Rule, see Ericksen [3]) then $r_i = R/3$, $i = 1,2,3$, but this may not correspond to minimal energy. To describe the situation, it is convenient to introduce $\phi_i = r_i - R/3$. Then, because of the special form of the potential $v(r)$ (see Fig.2) the Euler-Lagrange equations $v'(r_i) = const$ for $i = 1,2,3$ have at most two different solutions $r_i \neq r_j$ and one can always assume $\phi_1 = \phi_2 = \phi$ and $\phi_3 = -2\phi$ up to trivial permutations. This introduces the order parameter ϕ measuring the deviation from the Cauchy-Born Rule. There are essentially two different possibilities: $\phi = 0$ (trivial solution) and $\phi \neq 0$ ("fractured" solution). The behavior of the order parameter $\phi(R/3)$ along the nontrivial branch is shown in Fig. 3a; one can show that as $R \to \infty$ either one spring breaks, which means $\phi \to r_0 - R/3$ or two springs break and $-2\phi \to r_0 - R/3$.



(a) (b)

Fig. 3

A bifurcation from the trivial solution $\phi \equiv 0$ takes place at r_*, where the "spinodal point" r_* is defined by $v''(r_*) = 0$. The trivial branch is stable for $0 \le R/3 \le r_*$ and it corresponds to a global minimum for $0 \le R/3 \le \bar{r}$, where $\bar{r} < r_*$ satisfies $2v(\bar{r} + \phi(\bar{r})) + v(\bar{r} - 2\phi(\bar{r})) = 3v(\bar{r})$. The nontrivial lower branch in Fig.3a is stable for $r^* < R/3 < \infty$, where $r^* < \bar{r}$ satisfies $-2v''(r^* - 2\phi^*) = v''(r^* + \phi^*)$ and $v'(r^* - 2\phi^*) = v'(r^* + \phi^*)$. This corresponds to a global minimum of the energy (3.1) for $\bar{r} < R/3 < \infty$. The energies of the stable and unstable branches are shown in Fig.3b together with a sketch of a typical energy level set configuration in barycentric coordinates for a given value of $R/3 > r^*$.

One can see that contrary to the case of continuum model discussed in Sec.2, the discrete model predicts that the crack is incipient at the finite tension $v'(r_*)$; in addition the energy of the completely broken lattice at $R \to \infty$ is different from zero. Although states with multiple cracking are now unstable, the minimizer is still non unique in that the particular two atoms that become separated is undetermined. This nonuniqueness could, of course, be further narrowed, if an interaction between the next to nearest neighbors was taken into account or explicit imperfections were introduced.

4. FRACTURE IN THE DISCRETE SYSTEM OF MANY ATOMS

Now consider a one-dimensional lattice (chain) of N+1 atoms connected by N nonlinear springs. The energy of the system takes the form

$$V_N(r_1,...r_N) = \sum_{i=1}^{N} v(r_i;N), \tag{4.1}$$

where r_i, $i=1,...N$ are again the lengths of the deformed springs. The qualitative form of the energy $v(r_i;N)$ is sketched in Fig. 2; we explicitly specify here that the parameters of the potential (say A and r_0 in (3.2)) may depend on N. Suppose again that the total displacement is given, so that r_i satisfy the constraint

$$\sum_{i=1}^{N} r_i = R. \tag{4.2}$$

For the purpose of comparison with the continuum case, it is convenient to introduce the discrete analog of the strain gradients $w_i = r_i / r_0 - 1$. Without loss of generality one can assume that the undistorted chain has a unit length, therefore $r_0 = N^{-1}$. Then the total displacement of the chain is equal to $d = R - 1$, and the problem reduces to finding a (multivalued) function $V(d) = V(r_i(d))$, where $r_i(d)$, $i=1,...N$ correspond to the extremum of the energy (4.1) with the constraint (4.2).

As in the case of 4 atoms, at a given (nontrivial) branch of equilibrium the strains w_i can take only two values, say $w_*(d)$ and $w^*(d)$. Let $w_*(d) < w^*(d)$ so that w^* will be associated with the fractured region. Now the different branches of equilibrium can be parametrized by p $(0 \le p \le N)$ - the number of "overstretched" springs that have the larger of the two strains, $w^*(d)$. As the previous section shows, p and $N-p$ branches constitute two pieces of one single branch of the energy and they overlap for $p = N/2$ if N is even. Now it is natural to introduce the variable $\theta = p/N$ and reformulate the problem (4.1 - 4.2) for the given branch (given θ) as

$$F_N(\theta, w_*, w^*) = (1-\theta) f_N(w_*) + \theta f_N(w^*) \to extr, \tag{4.3}$$
$$(1-\theta) w_* + \theta w^* = d,$$

where

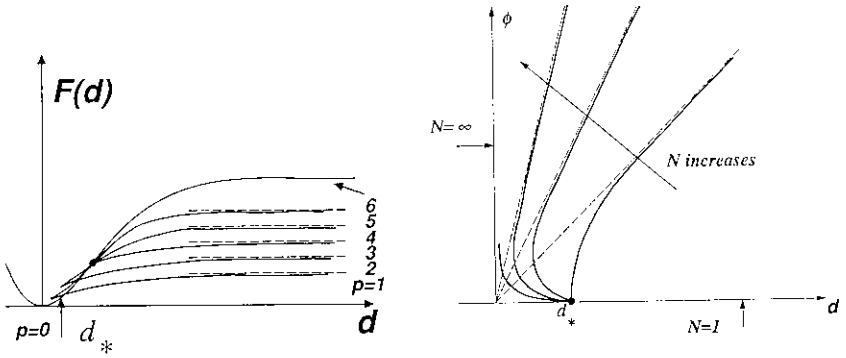
$$f_N(w) = N(v((w+1)N^{-1};N) - v(N^{-1};N)) \tag{4.4}$$

is the analog of the energy density used in the continuum description of Sec.2, and $F_N = V_N - V_0$ is the total elastic energy stored in the lattice. Here $V_0 = Nv(N^{-1};N)$ is the energy of the undistorted state which we assume to be a constant independent of N.

The solution of the problem (4.3 - 4.4) is illustrated in Fig. 4a for $N = 6$. The behavior of the energy branches is qualitatively similar to the case of 4 atoms: the trivial branch $(w_*(d) = w^*(d))$ is metastable until $d_* = r_* N - 1$ and the lowest nontrivial branch corresponds to $p = 1$ which means opening of a single crack. Fig. 4b shows the behavior of the order parameter $\phi = w^*(d) - d$ at the lowest energy branch for different N. Notice that at this branch $F_N \to -v(N^{-1};N)$ as $d \to \infty$. This means that complete breaking of the lattice requires finite energy. However in the limit $N \to \infty$ the "fracture energy" goes to zero since $v(N^{-1};N) \sim -N^{-1} \to 0$. We conclude that in the continuum limit the lattice can be broken without any expenditure of energy which is in agreement with the results of Sec.2. Moreover in the limit $N \to \infty$ the energy $F_N(N^{-1}, w_*(d), w^*(d))$ of the lowest branch ($p = 1$) approaches the convexification of the function

$$f(w) = \lim_{N\to\infty} f_N(w),$$

which is sketched in Fig. 1b. Obviously we again obtained a material that does not support tension.



(a) (b)

Fig. 4

5. SEPARATION OF SCALES

The disappearance of the fracture energy in the continuum limit is due to the fact that there is no internal length scale in the theory so at the end we are breaking infinitesimally small (and weak) springs. At the same time fracture is well known to be a size dependent phenomenon; the adequate continuum theory must therefore contain a small parameter with the scale of length. It should also be compatible with the results of the discrete model for large but finite N; in particular, one would like the energy of the global minimizer to reproduce the lowest energy branch from Fig. 4a. That essentially means: the trivial state is at least a local minimizer for $d \le d_*$, the state with the single localized fracture is stable beginning from some $d^* < d_*$ and the fracture energy is finite. The last assumption means $F(d) \to \gamma$ as $d \to \infty$, where $F(d)$ is the energy of the global minimizer and $\gamma > 0$ is the fracture energy. This brings a length scale into the theory since the trivial state is characterized by a parameter with the dimension of energy per unit length (say, elastic modulus), while γ has a dimension of energy (both per unit cross-sectional area).

To implement these ideas, consider our lattice with N springs and suppose that $r_0 = \varepsilon$, where ε is small but finite "length." It is in fact a nondimensional parameter since we already nondimensionalized the problem by taking $r_0 N = 1$, so now $N = \varepsilon^{-1}$. Since the zero approximation in ε leads to the "naive" continuum theory of Sec.2, the question arises what will be the asymptotic theory of the order ε.

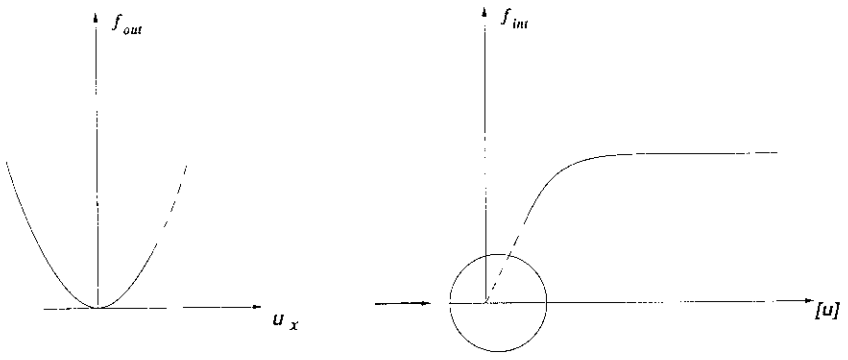
As we know, the discrete theory exhibits localization at the scale of ε, therefore it is natural to use different descriptions inside and outside the boundary layers (cracks). Thus, outside the fractured zone, variables w_i converge to $w = u_x$, while inside w_i diverges as ε^{-1} making it natural to define a new variable $[u]_i = \varepsilon w_i$ which describes a discontinuity of the displacement field at the site of the i-th fracture. Then it is straightforward to identify u_x with the "smaller" strain w_* and $[u]\varepsilon^{-1}$ with the "larger" strain w^* from Sec. 4. This means a separation of the slow and fast variables since $w^* >> 1$ and $w_* << 1$. Now, following (4.3) we represent the energy by two terms describing the behavior inside and outside the boundary layers

$$F = \int_0^1 f_{out}(u_x)dx + \varepsilon \sum_{i=1}^{k} f_{int}([u]_i \varepsilon^{-1}). \tag{5.1}$$

In (5.1) the displacement field $u(x)$ is assumed to be discontinuous in k (unknown) points. Now the constraint (4.4) can also be written as a sum of the two terms

$$\int_0^1 u_x dx + \varepsilon \sum_{i=1}^{k} ([u]_i \varepsilon^{-1}) = d. \tag{5.2}$$

The problem (5.1 - 5.2) represents a particular kind of the classical "cohesive zone" model (Barenblatt [2]). In order to proceed we need to choose two new functions $f_{out}(u_x)$ and $f_{int}([u]\varepsilon^{-1})$.



(a) **(b)**

Fig. 5

Since w_* is "small," only the portion of the energy function $f(w)$ from (4.4) will be relevant for the outer solution and one can identify $f_{out}(\cdot)$ with the fragment of the curve $f(\cdot)$ around $w = 0$. For example we can take a quadratic approximation (see Fig 5a) remembering that for large strain ($u_x >> 1$) the function $f_{out}(u_x)$ is not defined. Now, for the inner expansion, the only relevant portion of the energy function will be the one

where w^* is defined, so we can identify $f_{int}(\cdot)$ with the fragment of the curve $f(\cdot)$ at large w (see Fig 5b). Then as $q \to \infty$ we have $f_{int}(q) \to v(N^{-1};N) = \varepsilon V_0$; therefore one can set $\gamma = \varepsilon V_0$, which is in agreement with the idea that the small parameter ε measures the ratio of surface to elastic energy. Notice that γ is a product of a small and a large number. At $q \sim 1$ ($[u] \sim \varepsilon$) where the inner and outer expansions overlap, the function $f_{int}(q)$ is not defined. We shall impose the obvious unilateral constraint $q \geq 0$ which implies infinite potential barrier at $q = 0$. It can also be shown that if we want the trivial solution to be stable for sufficiently small d we must require $f_{int}(q) \sim q^{\alpha}$ around $q = 0$ with $0 \leq \alpha \leq 1$ (in classical Griffith's fracture mechanics $f_{int}(q) \equiv \gamma$, which means $\alpha = 0$).

Notice that this approach allows us to describe formation of a crack as a (subcritical) bifurcation at finite tension. In fact, consider an equilibrium configuration with a single crack and a constant strain outside. Then the original problem (5.1 - 5.2) reduces to

$$F(s,q) = f_{out}(s) + \varepsilon f_{int}(q) \to extr, \tag{5.3}$$

$$s + \varepsilon q = d. \tag{5.4}$$

Suppose for determinacy that the "convex" part of the energy is quadratic: $f_{out}(s) = \frac{1}{2}Es^2$. Then it is not hard to choose the "concave" part $f_{int}(q)$ (see Fig.5b) in such a way that the equilibrium curve $F(d) = F(s(d),q(d))$ will have a desirable behavior (Fig.6). If, for example, we assume $f_{int}(q) \sim \mu q$ at small q (which means $\alpha = 1$), the trivial configuration with $F(d) = \frac{1}{2}Ed^2$ is metastable for $d \leq a_*$ where $a_* \sim \mu / E$.

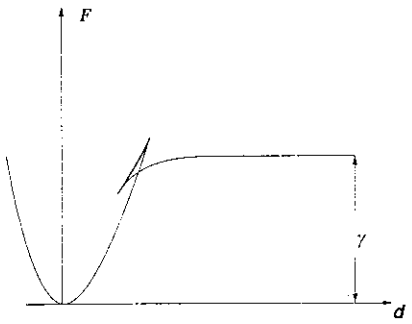


Fig. 6

6. MULTIPLE CRACKING

Although our discrete model predicts the instability of the lattice with an opening of a single crack, it is well known from experiment that multiple fractures are common and a system of microcracks may develop. One reason for multiple cracking is the

incompatibility of a single - crack state with the boundary conditions. This is the case when displacements are prescribed on the boundary of the body (hard device) or when the brittle body is surrounded by an elastic matrix (like in polycrystals). The situation is very similar in the theory of martensitic phase transformations where the phase mixtures originate from the incompatibility of a single phase state with the constraints. In that sense multiple cracking is a direct analog of twinning.

Although this effect is at least two-dimensional, in the one dimensional setting the adequate constraint can be achieved through the introduction of a deformable foundation. In its simplest variant that would mean the following modification of the main functional (5.1) :

$$F = \int_0^1 f_{out}(u_x)dx + \varepsilon\sum_{i=1}^{k} f_{int}([u]_i\varepsilon^{-1}) + \beta\int_0^1 (u-h(x))^2 dx \,, \tag{6.1}$$

where $h(x)$ is a prescribed deformation of the foundation and parameter β measures the stiffness of the non interacting linear bonds between the bar and the foundation. Since the functional (6.1) is no longer translationally invariant, one has to specify displacements of the ends of the bar in addition to the total deformation, for example

$$u(0) = -d/2, u(1) = d/2 \cdot \tag{6.2}$$

The function $h(x)$ may or may not depend on d; the situation is already nontrivial if $h(x) \equiv 0$. If the fracture energy γ is equal to zero (if $\varepsilon = 0$), the solution of the minimization problem for the functional (6.1) with the boundary conditions (6.2) represents an infinitely fine distribution of infinitesimal cracks. If $\gamma \neq 0$, one would expect the "quantization" effect when the number of cracks changes in finite discrete steps as we change d, γ or β. This phenomenon has been recently observed by Truskinovsky and Zanzotto [5] in the case of phase transformations (double well energy) in a slightly different setting, when the "fracture energy" term in (6.1) is substituted by the "surface energy" term $\varepsilon^2\int u_{xx}^2 dx$.

If the distribution of the cracks is sufficiently fine one can think about homogenized description and try to approximate the discrete sums in (5.1, 5.2) by integrals. By assuming periodicity at least away from the boundaries, we can always choose representative material particle (homogenization cell) in such a way that it contains only one crack. Then the minimization problem inside this cell reduces to (5.3-5.4) where s is the microstrain, q is a local measure of displacement discontinuity and d is a macrostrain. In terms of the homogenized description the following identification is natural

$$d = u_x,$$

where $u(x)$ is the smooth field of macrodisplacements. If we now define the local measure of damage (order parameter) as $\phi = q$, we can introduce the homogenized energy per unit length by rewriting (5.3) as

$$g(u_x, \phi) = f_{out}(u_x - \varepsilon\phi) + \varepsilon f_{int}(\phi) \cdot$$

Then the minimization problem for the fields $u(x)$ and $\phi(x)$ takes the form

$$G\{u(x),\phi(x)\} = \int g(u_x,\phi)dx \to \inf, \tag{6.3}$$

$$\int u_x dx = \Delta. \tag{6.4}$$

The phenomenological theory of this type has recently been suggested by Del Piero [6]. It is not hard to see that for our choice of f_{int} and f_{out}, the equilibrium function $G(\Delta)$ calculated for the homogenous fields u_x and ϕ is not convex exhibiting "softening" behavior (see Fig. 6). This leads again to localization phenomena and to regularize the homogenized theory one would have to introduce another length scale δ, such that $\varepsilon << \delta << 1$; this parameter now characterizes the distance between the interacting microcracks. Then the theory providing the finite size zones of localized damage can be obtained by adding to the functional (6.3) another term which describes crack interactions, for instance $\delta^2\int\phi_x^2 dx$. The corresponding "Timoshenko-type" model gives an interesting example of elasticity with strong (integral) spatial nonlocality.

ACKNOWLEDGMENT

Helpful discussion of this paper with R. Fosdick is gratefully acknowledged. This work was supported by the National Science Foundation Grant DMS 9501433.

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