

Some Recent Developments in Nonlinear Elasticity and its Applications to Materials Science

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1 Introduction

Vital to a proper understanding of mathematical models of nature is knowledge of the possible singularities possessed by solutions of the governing equations together with physical interpretations of these singularities. The underlying theme of this article will be to discuss this within the context of elasticity theory, for which such knowledge has important implications for the understanding of the behaviour of materials. In elasticity theory materials are characterised by their corresponding free-energy functions, and so we need to know how different assumptions on the free-energy function can give rise to various types of singularity in the solution. This philosophy might lead one also towards a strategy for proving that solutions for certain partial differential equations (PDE's) are smooth, namely to classify the possible singularities of a class of such equations and to identify hypotheses on the form of the equations to eliminate each kind of singularity in turn. This is *not* how regularity theory for PDE's is generally approached, but we will see some hints that such a strategy might be viable in the future.

We consider three main topics:

- (a) 'Mathematically well-behaved materials', i.e. the study of a special class of free-energy functions leading to the existence of energy minimisers with mathematically desirable properties, and including some commonly used models of particular materials.
- (b) Fracture and its mathematical description.
- (c) Materials that can undergo phase transformations.

We shall see that the description of (b) and (c) cannot be subsumed under (a) because of the nature of the corresponding singularities.

2 Elasticity and Energy Minimisation

We begin by reviewing how to describe the deformation of an elastic body. We consider **only the static case**, that is, only deformations independent of time are considered, and no attempt is made to describe the dynamical process by which these deformations arise. This is partly for simplicity, but largely because our understanding of dynamics is, by comparison, very limited. Let $\Omega \subset \mathbb{R}^n$ represent the reference configuration of an elastic body which we use to label its material points. Using the Lagrangian description, the position of a point $x \in \Omega$ in a typical deformed configuration is denoted by $y(x) \in \mathbb{R}^n$ (see Fig. 1). Thus $y : \Omega \rightarrow \mathbb{R}^n$. Of course, the cases of interest are $n = 1, 2$ or 3. The gradient of y at x is written $Dy(x)$, and can be identified with the $n \times n$ matrix of partial derivatives $(\frac{\partial y_i}{\partial x_j}(x))$.

The material will be assumed homogeneous, so that its mechanical response (i.e. the stress corresponding to a given strain) is independent of the point x . Note that this is more restrictive than saying that Ω is occupied by the same material at each point, due to the possibility of pre-existing stresses.

The first question we consider is concerned with the choice of functions which should be used for a suitable mathematical model of deformations.

To be physically acceptable a deformation y should be *invertible*. This is essentially to avoid interpenetration of matter. However we still might want to allow cases where self-contact occurs. For example the deformation of a bar illustrated in Fig. 2 is an acceptable deformation, although it is not invertible on $\bar{\Omega}$. Also cases where y is invertible in Ω except on a set of measure zero could be considered (e.g. when the inverse image of a point is a line or a surface). In order that the deformation y be orientation preserving and have the same orientation as in the reference configuration we require that

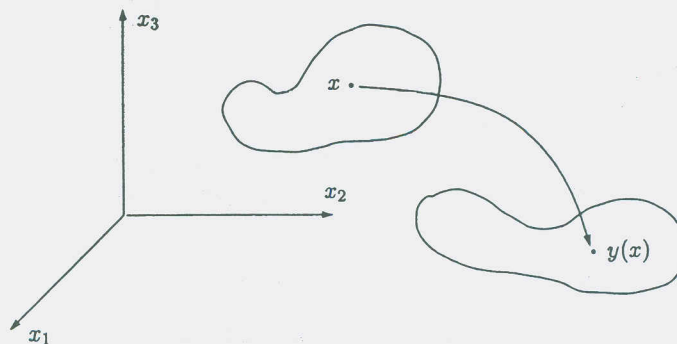


Figure 1: Description of deformation of a three-dimensional elastic body.

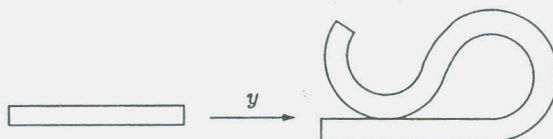


Figure 2: A deformation which is invertible on Ω but not on $\bar{\Omega}$.

$$\det Dy(x) > 0 \tag{2.1}$$

almost everywhere (a.e.) in Ω . If $y \in C^1(\Omega; \mathbb{R}^n)$, (2.1) implies local invertibility, this being a consequence of the Inverse Function Theorem. However local invertibility does not imply global invertibility as the deformation of a bar illustrated in Fig. 3 shows.

If $y \notin C^1(\bar{\Omega}; \mathbb{R}^n)$ then (2.1) does not even imply local invertibility. As an example consider the mapping $y : (r, \theta) \mapsto (r, 2\theta)$ of the unit disc in \mathbb{R}^2 to itself. It is easily checked that the gradient is bounded a.e. and that its determinant is a positive constant. However y is not invertible in any neighbourhood of the origin. A key tool for proving global, and even local, invertibility is *degree theory*. For various results see [10, 26, 33, 44, 65, 68].

Suppose now that Ω is a bounded, open connected set with a Lipschitz boundary $\partial\Omega$ (i.e. each point $x \in \partial\Omega$ has a neighbourhood in which $\partial\Omega$ can be represented as the graph of a Lipschitz function and in which Ω lies on one side of $\partial\Omega$). Let $\partial\Omega_1 \subset \partial\Omega$ be a portion of the boundary with $\mathcal{H}^{n-1}(\partial\Omega_1) > 0$, where \mathcal{H}^{n-1} denotes $(n-1)$ -dimensional Hausdorff measure (i.e. surface area). We consider the boundary condition

$$y|_{\partial\Omega_1} = f \tag{2.2}$$

for a given mapping $f : \partial\Omega_1 \rightarrow \mathbb{R}^n$. We impose no boundary conditions on the remaining part of the boundary $\partial\Omega \setminus \partial\Omega_1$. For the variational problem we

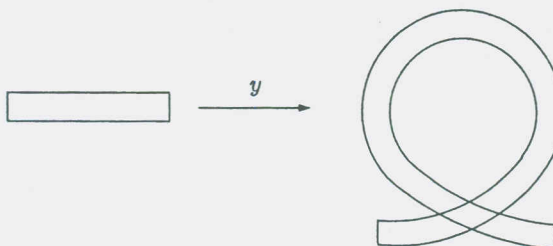


Figure 3: A locally invertible deformation that is not globally invertible.

consider this will formally correspond to requiring that the applied traction vanish on $\partial\Omega \setminus \partial\Omega_1$. The elastic energy corresponding to the deformation y is defined as

$$I(y) = \int_{\Omega} W(Dy) \, dx, \quad (2.3)$$

where $W : M^{n \times n} \rightarrow [0, \infty]$ is the free-energy (or stored-energy) function and $M^{n \times n}$ denotes the space of real $m \times n$ matrices. The assumption that $W \geq 0$ is made simply for convenience (it is natural to assume that W is bounded below, and adding a constant to W does not change the problem). We assume that $W(A)$ is finite and continuous for $\det A > 0$, and that

$$W(A) \rightarrow \infty \quad \text{as} \quad \det A \rightarrow 0+, \quad (2.4)$$

which physically means that an infinite amount of energy is required to crush the material down to zero volume. Consistent with the constraint (2.1) we suppose that $W(A) = \infty$ for $\det A \leq 0$. Thus W is continuous with respect to the natural topology on $[0, \infty] = [0, \infty) \cup \{\infty\}$.

Question. *Does there exist a \bar{y} minimising I subject to the boundary condition (2.2)?*

The above question is imprecise since the class of admissible functions is not clearly specified. Also it is not clear what we mean by Dy . These issues can be explored by considering the underlying physics of the problem. In general enlarging the set of admissible functions can change the nature of the solution. It may result in the infimum of the energy functional changing (the *Laurentiev phenomenon*) and affect whether or not the infimum is attained. It is thus important to assess whether or not a given set of admissible functions has a physical justification. For example the absolute minimum of the energy

$$I(y) = \int_0^1 y'^2 \, dx$$

subject to the boundary condition $y(0) = 0$, $y(1) = 1$ is attained by the well-known Cantor function when y' is interpreted as the limit of a difference quotient, with minimum value zero. However such a function would usually be regarded as too irregular to represent an acceptable physical deformation. Among more regular functions, such as we use below, the minimum value is 1, attained by the function $y(x) = x$. Other more surprising examples can be found in [16]. In our case we make the set of admissible functions precise by using the standard notion of Sobolev spaces (see, for example, [2, 25, 32, 52, 54]).

For $1 \leq p \leq \infty$ define the Sobolev space $W^{1,p} = W^{1,p}(\Omega; \mathbf{R}^n)$ to be the set of equivalence classes of mappings $y : \Omega \rightarrow \mathbf{R}^n$ which together with their first order weak derivatives belong to L^p . This means that

$$\|y\|_{1,p} = \left(\int_{\Omega} (|y|^p + |Dy|^p) \, dx \right)^{\frac{1}{p}} < \infty \quad \text{if } 1 \leq p < \infty,$$

$$\|y\|_{1,\infty} = \operatorname{ess\,sup}_{x \in \Omega} (|y(x)| + |Dy(x)|) < \infty,$$

where $Dy = \left(\frac{\partial y_i}{\partial x_j}\right)$ denotes the matrix of first order weak partial derivatives of y , defined to satisfy

$$\int_{\Omega} \frac{\partial y_i}{\partial x_j} \varphi \, dx = - \int_{\Omega} y_i \frac{\partial \varphi}{\partial x_j} \, dx \quad \text{for all } \varphi \in C_0^\infty(\Omega). \quad (2.5)$$

In (2.5) $C_0^\infty(\Omega)$ denotes the space of infinitely differentiable real-valued functions on Ω which vanish outside a compact subset of Ω . We can now pose our question more precisely by setting

$$\mathcal{A} = \{y \in W^{1,1} : y|_{\partial\Omega_1} = f, \quad I(y) < \infty\}. \quad (2.6)$$

In (2.6) the boundary condition is to be understood in the sense of *trace* (for the precise meaning see the general references cited above).

Question (precise formulation). *Assume that \mathcal{A} is not empty. Does there exist a function $\bar{y} \in \mathcal{A}$ minimising I ?*

3 Mathematically Well-Behaved Materials

In this section we consider a class of materials for which a positive answer to the above question can be given, and highlight some limitations of the existing theory.

3.1 Statement of the existence theorem

Suppose $n = 3$ and that

(H1) W is *polyconvex* i.e. there exists a convex function $g : M^{3 \times 3} \times M^{3 \times 3} \times (0, \infty) \rightarrow \mathbf{R}$ such that $W(A) = g(A, \operatorname{cof} A, \det A)$ for all $A \in M^{3 \times 3}$ with $\det A > 0$;

(H2) $W(A) \geq c_0(|A|^p + |\operatorname{cof} A|^q) - c_1$, where $c_0 > 0$, $p \geq 2$, $q \geq \frac{3}{2}$.

Here $\operatorname{cof} A$ denotes the matrix of cofactors of A . Then we have the following result.

Theorem 1 *Let (H1) and (H2) hold. Then there exists \bar{y} minimising I in \mathcal{A} . Furthermore $\det D\bar{y}(x) > 0$ for a.e. $x \in \Omega$.*

3.2 Commentary

Theorem 1 is of the type first proved in Ball [8] under somewhat stronger growth hypotheses. It was refined by Ball & Murat [17], who assumed that $q \geq \frac{p}{p-1}$, and then by Müller, Qi & Yan [48] in the version stated here.

The theorem avoids the blunder of assuming W to be convex. This is not a physically realistic assumption. For example, a consequence of convexity of W would be that any equilibrium configuration (solution of the Euler-Lagrange equation) is an absolute minimiser, in particular ruling out buckling phenomena. Also note that the set $M_+^{3 \times 3} = \{A \in M^{3 \times 3} : \det A > 0\}$ is not convex, so that W cannot both be convex and satisfy (2.4).

To give examples of materials satisfying (H1), (H2) and (2.4), let us first look at some general properties of the free-energy function. First, W should satisfy the frame-indifference condition

$$W(A) = W(RA) \quad \text{for all } A \in M_+^{3 \times 3}, \quad R \in SO(3).$$

This condition reflects the fact that rigid rotations of a body do not change its energy, and is assumed to hold for all materials.

The symmetry of the material is expressed by the condition

$$W(A) = W(AR) \quad \text{for all } A \in M_+^{3 \times 3}, \quad R \in \mathcal{S},$$

where we will assume that the symmetry group \mathcal{S} of the material is a subgroup of $SO(3)$. A particular case is when the material has no preferred grain. This corresponds to the case $\mathcal{S} = SO(3)$, and the material is called *isotropic*. Using the polar decomposition theorem it can be shown that W is frame-indifferent and isotropic if and only if W has the representation

$$W(A) = \Phi(v_1, v_2, v_3)$$

for $\det A > 0$, where v_1, v_2 and v_3 are the singular values of A (i.e. the eigenvalues of $(A^T A)^{\frac{1}{2}}$) and Φ is symmetric with respect to permutations of the v_i . Writing

$$\begin{aligned} \phi(\alpha) &= v_1^\alpha + v_2^\alpha + v_3^\alpha - 3, \\ \psi(\beta) &= (v_2 v_3)^\beta + (v_3 v_1)^\beta + (v_1 v_2)^\beta - 3, \end{aligned}$$

then the well-known Ogden materials ([56, 57]) have the form

$$\Phi(v_1, v_2, v_3) = \sum_{i=1}^M a_i \phi(\alpha_i) + \sum_{i=1}^N b_i \psi(\beta_i) + h(v_1 v_2 v_3),$$

where $a_i > 0$, $b_i > 0$, $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_M \geq 1$, $\beta_1 \geq \beta_2 \geq \dots \geq \beta_N \geq 1$, and where $h : (0, \infty) \rightarrow [0, \infty)$ is convex, with $h(\delta) \rightarrow \infty$ as $\delta \rightarrow 0$. These free-energy functions satisfy (H1) and (2.4). If $\alpha_1 \geq 2$ and $\beta_1 \geq \frac{3}{2}$ then they

also satisfy (H2). For appropriate values of the constants good fits can be obtained for the behaviour of rubber-like materials.

In order to place the polyconvexity hypothesis (H1) in perspective we consider some related classes of free-energy functions. We say that W is *rank-one convex* if and only if it is convex in every rank-one direction, that is $t \mapsto W(A + t\lambda \otimes \mu)$ is a convex function of t for every $A \in M^{3 \times 3}$ and $\lambda, \mu \in \mathbf{R}^3$. If $t \mapsto W(A + t\lambda \otimes \mu)$ is strictly convex for $t \geq 0$ whenever $A, A + \lambda \otimes \mu \in M_+^{3 \times 3}$ we say that W is *strictly rank-one convex*.

In the case when $W \in C^2(M_+^{3 \times 3})$, rank-one convexity is equivalent to the Legendre-Hadamard condition

$$\frac{d^2}{dt^2}W(A + t\lambda \otimes \mu)|_{t=0} \geq 0 \quad \text{for all } A \in M_+^{3 \times 3}, \lambda, \mu \in \mathbf{R}^3,$$

that is

$$\frac{\partial^2 W}{\partial A_{ij} \partial A_{kl}}(A) \lambda_i \mu_j \lambda_k \mu_l \geq 0 \quad \text{for all } A \in M_+^{3 \times 3}, \lambda, \mu \in \mathbf{R}^3, \quad (3.1)$$

where we have used the summation convention. If strict inequality holds in (3.1) whenever λ and μ are nonzero, then W is said to be *strongly elliptic*.

We say that W is *quasiconvex* if

$$\int_E W(Dv) dx \geq \int_E W(A) dx$$

for every bounded open set $E \subset \mathbf{R}^3$ and $v \in C^1(E; \mathbf{R}^3)$ with $v = Ax$ in a neighbourhood of ∂E . It can be shown by a scaling argument that the definition of quasiconvexity is independent of E . The definitions of polyconvexity, rank-one convexity and quasiconvexity extend in the obvious way to arbitrary dimensions, i.e. to integrands $W : M^{m \times n} \rightarrow [0, \infty]$. The following implications then hold:

$$\text{polyconvexity} \implies \text{quasiconvexity} \implies \text{rank-one convexity.}$$

In particular all the above notions coincide with the usual convexity when either $n = 1$ or $m = 1$.

The importance of rank-one matrices lies in the fact that a deformation $y \in W^{1,1}(\Omega; \mathbf{R}^m)$ can have its gradient equal to A and B respectively above and below a specific $(n - 1)$ -dimensional hyperplane intersecting Ω if and only if the difference $A - B$ is a rank-one matrix. To justify this statement, known as the *Hadamard jump condition*, let y be such that

$$Dy = \begin{cases} A & \text{if } x \cdot \mu > k, \\ B & \text{if } x \cdot \mu < k, \end{cases}$$

for some $k \in \mathbf{R}$ and unit vector $\mu \in \mathbf{R}^n$. Applying the continuity on the interface (the existence of a continuous representative follows from the boundedness of Dy and the Sobolev Embedding Theorem), we obtain $C\mu^\perp = 0$ whenever $\mu^\perp \cdot \mu = 0$, where $C = A - B$. Since

$$\begin{aligned} (C - C\mu \otimes \mu)\mu &= 0, \\ (C - C\mu \otimes \mu)\mu^\perp &= 0 \quad \text{for } \mu^\perp \cdot \mu = 0, \end{aligned}$$

it follows that $C = C\mu \otimes \mu$ and therefore $A - B = \lambda \otimes \mu$ for some $\lambda \in \mathbf{R}^m$. Conversely if $A - B = \lambda \otimes \mu$ one can easily find a deformation whose gradient is equal to A and B respectively below and above an $(n - 1)$ -dimensional hyperplane with normal μ . This construction will be used frequently in Section 5 below.

It would be less restrictive in Theorem 1 to replace the polyconvexity of W by quasiconvexity. There are various results in the calculus of variations of this type following from the pioneering work of C.B. Morrey [45, 46] (see, for example, [1, 43]). However the assumptions made are not consistent with the growth conditions of nonlinear elasticity. Quasiconvexity is a difficult condition to verify as it is not defined in a pointwise manner, and no equivalent pointwise condition (i.e. one depending on W and its derivatives at an arbitrary matrix) is known. For over 40 years it was a conjecture arising out of the work of Morrey that quasiconvexity was equivalent to rank-one convexity. However in 1992 V. Šverák [66] produced a counterexample for a quartic $W = W(Dy)$ for the case when $y : \Omega \subset \mathbf{R}^n \rightarrow \mathbf{R}^m$ and $n \geq 2, m \geq 3$. The case when $m = n = 2$ remains open, and there is some evidence that rank-one convexity might imply quasiconvexity in this case (see [27, 28, 59, 60]).

Theorem 1 (and many others similar to it by nature) guarantees the existence of at least one (global) minimiser. However it does not say anything about how smooth such a minimiser is. In particular one is interested to know whether or not the Euler-Lagrange equations are satisfied. To derive the Euler-Lagrange equations we need to calculate the first variation of I . Let $\varphi : \Omega \rightarrow \mathbf{R}^3$ be smooth with $\varphi|_{\partial\Omega_1} = 0$. Then $\bar{y} + t\varphi \in \mathcal{A}$ for any $t \in \mathbf{R}$ and so

$$\frac{d}{dt}I(\bar{y} + t\varphi)|_{t=0} = \int_{\Omega} D_A W(D\bar{y}) \cdot D\varphi \, dx = 0 \quad (3.2)$$

provided this derivative exists and is given by the anticipated expression in (3.2). To justify this we need the existence of the limit

$$\lim_{t \rightarrow 0} \frac{1}{t} [I(\bar{y} + t\varphi) - I(\bar{y})] = \lim_{t \rightarrow 0} \int_{\Omega} \frac{1}{t} [W(D\bar{y} + tD\varphi) - W(D\bar{y})] \, dx, \quad (3.3)$$

where we assume that $W \in C^1(M_+^{3 \times 3})$ say. But it is not obvious how to pass to the limit inside the integral in (3.3) unless we have additional information on \bar{y} , so that for example the integrands are bounded pointwise by an integrable function (for the application of the Dominated Convergence Theorem).

This is the case if $\bar{y} \in W^{1,\infty}$ with $\det D\bar{y} \geq \varepsilon > 0$ for some $\varepsilon > 0$. However, the only readily available piece of information is that $I(\bar{y}) < \infty$. In fact there are one-dimensional counterexamples (see [16]) of minimisers which do not satisfy the corresponding Euler–Lagrange equation, even for elliptic polynomial integrands. The Euler–Lagrange equation is then an elliptic ordinary differential equation; weak solutions of such equations are smooth, but the minimisers are not. It is not known whether the minimiser \bar{y} given by Theorem 1 satisfies (3.2). However, it is possible to derive other weak forms of the Euler–Lagrange equation under supplementary growth hypotheses on W (see [12, 19]).

The condition of *strict rank-one convexity* is intimately related to the possible occurrence of the type of singularity we previously considered in which Dy jumps across a hyperplane. In fact (see [9]), under the very mild supplementary hypothesis that the integrand W has a minimiser, strict rank-one convexity is necessary and sufficient for the nonexistence of such singularities in solutions to the Euler–Lagrange equations.

The general question of whether the minimisers in Theorem 1 are smooth is unresolved. A well-known theorem of Evans [31] implies ‘partial regularity’ of minimisers \bar{y} of integrals of the form (2.3) with W satisfying a strict form of quasiconvexity, though again unfortunately under growth hypotheses inconsistent with (2.4). More precisely he proves that under his hypotheses \bar{y} is smooth off a closed set S of measure zero. Such a result would be very interesting for the minimisers in Theorem 1, especially if S were nonempty for physically reasonable W . The existence of points $x_0 \in S$ where $|D\bar{y}(x_0)| = \infty$ in some sense might, for example, have something to do with the onset of fracture, though as we discuss in Section 4, the energy functional I needs modification for actual fracture to be described. The counterexample of Nečas [53] shows that if \bar{y} is in fact smooth (so that S is empty) this must have something to do with either the special form of W or with special features of 3 (or low) dimensions. Even under the growth hypotheses of Evans essentially nothing is known about regularity up to the boundary.

For recent advances in the regularity theory of minimisers in elasticity see [18, 19, 20, 21, 34, 35, 64].

In Theorem 1 the minimisation was carried out in a space \mathcal{A} of deformations y satisfying the condition $\det Dy > 0$ a.e.. As we saw in Section 2 such deformations need not even be locally invertible, and to be physically realistic we should instead minimise over globally invertible deformations. In the case of pure displacement boundary conditions (i.e. $\partial\Omega_1 = \partial\Omega$) this turns out not to be a serious issue, since in fact the minimiser \bar{y} in Theorem 1 can be shown to be a homeomorphism provided the boundary data f is consistent with invertibility and provided somewhat stronger growth conditions are imposed on W (see [10, 65]). However, for mixed boundary conditions ($\partial\Omega_1 \neq \partial\Omega$) there is no escaping the need for a new approach, and one way is to proceed as in Ciarlet & Nečas [26]. However, there is much to be done before the true

complications of self-contact can be satisfactorily addressed.

4 Fracture and Cavitation

4.1 Towards a theory of fracture

Why and how do materials break? These are the questions studied in the important technological subject of *fracture mechanics*. By far the largest proportion of work in fracture mechanics concerns the possible extension and evolution of *pre-existing cracks* under different loadings. In contrast, comparatively little is said about fracture initiation. Although there are isolated rigorous treatments of parts of classical fracture mechanics (see, for example, [58]), from the mathematical perspective fracture mechanics is in a somewhat primitive state, reflecting the difficulty of considering (or eliminating from consideration on some rational basis) very complicated potential fracture patterns. There is perhaps now the beginnings of a more general and rigorous approach to be seen in the work on problems with 'free discontinuity sets' based on ideas of geometric measure theory (see [3, 4, 30, 51]). But there is a need to link these new ideas with classical work in fracture mechanics, a necessary preliminary to a more comprehensive theory.

A first mathematical difficulty which arises is that we cannot use Sobolev spaces to directly model fracture in general. In the typical fracture patterns illustrated in Fig. 4 the deformations y shown jump across a two-dimensional surface, and hence $y \notin W^{1,1}$.

Let us consider the static case. The idea in [3, 4, 30, 51] is to seek to minimise the modified energy

$$I(y, K) = \int_{\Omega \setminus K} W(Dy) dx + k\mathcal{H}^2(K), \quad k > 0, \quad (4.1)$$

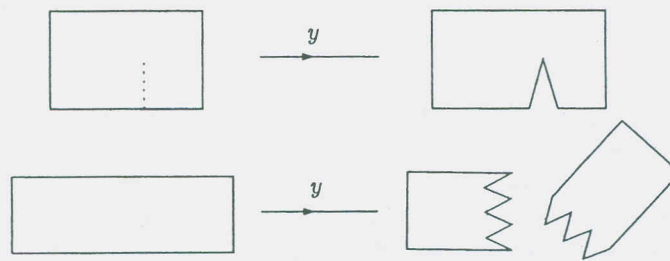


Figure 4: Examples of deformations y involving fracture: such deformations do not belong to Sobolev spaces.

subject to some boundary conditions. Here Ω and W are as before, and the new unknown K is the *crack set*. The second term is the simplest way to take into account the contribution of the surface energy due to the creation of cracks. Here $\mathcal{H}^2(K)$ denotes the two-dimensional Hausdorff measure of K and coincides with usual definitions of surface area for smooth sets K . The competing functions y are supposed to belong to $W^{1,1}(\Omega \setminus K; \mathbf{R}^3)$. This allows them to have a jump across the crack set.

The main difficulty here is that we want to minimise I without making any *a priori* assumptions on the set K . A key technical device introduced by Ambrosio & de Giorgi in [30, 3, 4] is to remove the dependence of the integral in (4.1) on K by using the space $SBV(\Omega; \mathbf{R}^3)$. This space is defined in terms of the space $BV(\Omega; \mathbf{R}^3)$ of mappings $y : \Omega \rightarrow \mathbf{R}^3$ of *bounded variation*, consisting of those $y \in L^1(\Omega; \mathbf{R}^3)$ whose gradient Dy is a bounded measure. This gradient can be decomposed as the sum of a part ∇y that is absolutely continuous with respect to 3-dimensional Lebesgue measure, and a singular part $D^s y$:

$$Dy = \nabla y \, dx + D^s y.$$

The singular part can be further decomposed as

$$D^s y = (y^+ - y^-) \nu_y \, d\mathcal{H}^2|_{S_y} + Cy,$$

where ν_y is the measure theoretic normal to the set of *jump points* S_y , y^\pm denote the traces of y on either side of S_y , and Cy is the *Cantor part* of Dy . $SBV(\Omega; \mathbf{R}^3)$ is now defined as consisting of those $y \in BV(\Omega; \mathbf{R}^3)$ whose Cantor part $Cy = 0$. We can now replace the problem of minimising (4.1) by that of minimising the associated functional

$$I(y) = \int_{\Omega} W(\nabla y) \, dx + k\mathcal{H}^2(S_y) \tag{4.2}$$

over a suitable subset of $SBV(\Omega; \mathbf{R}^3)$. There is now a considerable literature on existence and regularity of minimisers for functionals of the form (4.2) (see, for example, [5, 6, 24, 29]). However, from the point of view of applications to fracture mechanics a missing ingredient seems to be a calculation of a general variation for I about a given \bar{y} in the direction of a nearby y having a possibly very different set of jump points.

4.2 Cavitation

Cavitation is a common failure mechanism in polymers, such as rubber, characterised by the formation of (roughly spherical) holes (see [36]). Fortunately it is possible to express cavitation in Sobolev spaces with an unmodified energy functional

$$I(y) = \int_{\Omega} W(Dy) \, dx. \tag{4.3}$$

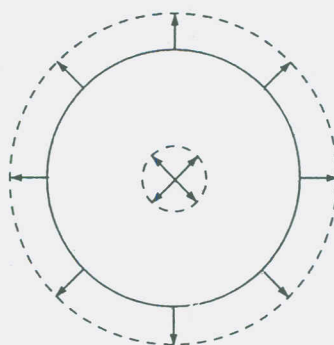


Figure 5: Radial cavitation.

In the simplest situation of radial cavitation, a hole forms at the centre of a ball whose outer boundary is radially displaced (see Fig. 5).

The corresponding deformation y is discontinuous, since it maps a solid ball into one with a hole. For such a deformation to have finite energy (4.3) W must have restricted growth. In fact, if the material is 'strong', namely

$$W(A) \geq C(1 + |A|^\gamma), \quad A \in M_+^{3 \times 3} \quad (4.4)$$

for some $\gamma > 3$, then it follows immediately from the Sobolev Embedding Theorem that any deformation y with $I(y) < \infty$ is continuous. Thus *cavitation type singularities* cannot occur in strong materials.

Let Ω be the open ball $B = \{x \in \mathbb{R}^3 : |x| < 1\}$ and consider radial deformations of the type

$$y(x) = \frac{r(|x|)}{|x|}x. \quad (4.5)$$

Such deformations y map spheres to spheres and displace points of B in the direction of their position vectors with respect to the centre of B . We assume that the material is isotropic. The question is now whether or not there exists any radial minimiser whose corresponding r in (4.5) satisfies $r(0) > 0$. After some calculations it can be shown that the singular values of Dy are

$$v_1 = r'(|x|), \quad v_2 = v_3 = \frac{r(|x|)}{|x|}.$$

Therefore restricting to the class of radial functions $I(y) = \int_B W(Dy) dx$ takes the form

$$E(r) = 4\pi \int_0^1 R^2 \Phi(r', r/R, r/R) dR.$$

We can try to minimise E over the set of admissible functions

$$\mathcal{A}_\lambda = \{r \in W^{1,1}(0, 1) : r' > 0 \text{ a.e., } r(1) = \lambda, r(0) \geq 0\},$$

where the parameter λ represents the boundary displacement (one can formulate the traction problem in a similar fashion).

Consider now the special free-energy function

$$\Phi(v_1, v_2, v_3) = v_1^\alpha + v_2^\alpha + v_3^\alpha + h(v_1 v_2 v_3), \quad 1 < \alpha < 3, \quad (4.6)$$

where h is smooth and satisfies

$$h'' > 0, \quad \lim_{\delta \rightarrow \infty} \frac{h(\delta)}{\delta} = \lim_{\delta \rightarrow 0^+} h(\delta) = \infty.$$

Note that this free-energy function satisfies (H1) but not (H2) for the given range of α .

It can be shown that for λ less than a critical value λ_{cr} the trivial solution $r(R) = \lambda R$ (i.e. $y(x) = \lambda x$) is the only (global) minimiser of E . However if $\lambda > \lambda_{cr}$ there is an exchange of stability and a nontrivial cavitating solution r_λ with $r_\lambda(0) > 0$ becomes the global minimiser, the trivial solution becoming unstable. The bifurcation diagram Fig. 6 shows this.

The above example has been studied for a wider range of W in [11] (for different methods see [61, 63]). There it is shown that the minimisers r_λ satisfy the Euler-Lagrange equations and hence provide singular weak solutions to the 3D equations of nonlinear elastostatics. However it is not known in general whether the radial deformations still remain minimisers when one considers variations that are not radially symmetric, or whether λ_c gives the correct critical boundary displacement when arbitrary nonradial deformations are allowed. If the growth of $W(A)$ is less than quadratic in A then it has been shown by James & Spector [40] that for certain free-energy functions further reduction of energy is possible by introducing cylindrical voids along radial lines. For a recent review of cavitation in elastic materials see [39].

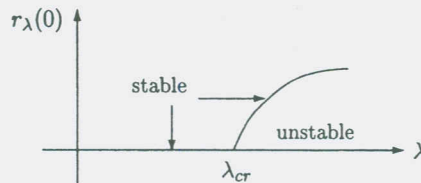


Figure 6: Bifurcation of the radial minimiser r_λ from the trivial solution $r(R) = \lambda R$.

The phenomenon of cavitation is a striking illustration of the fact that the function space chosen is *part of the mathematical model*. If we choose to minimise in, say, $W^{1,p}$ for $p > 3$ then the unique minimiser y of I subject to $y|_{\partial B} = \lambda x$ is $\bar{y}(x) = \lambda x$ (because W given through (4.6) is quasiconvex) and cavitation is not predicted. For general formulations of this kind of minimisation see Giaquinta, Modica & Souček [38] and the simplification of Müller [47]. If we choose to minimise in the smaller spaces considered in [38] (which has the advantage of a general 3D existence theory), the only way to recover cavitation is to suppose that the body already possesses small pre-existing holes. Although such holes do not seem to have been observed, they were postulated in [36] as being the precursors of cavitation. Since there are experiments [55, 37] in which cavitation appears at well-defined and repeatable geometric locations (see [62] for a corresponding theory based on our model above), in order to use the spaces in [38] we would need to assume that the pre-existing holes permeate the body, leading to a reference domain Ω with very complicated geometrical structure. This makes these spaces unattractive for modelling cavitation. Sivaloganathan [61] considered the case when the reference domain contains a pre-existing hole of radius ε , with a zero traction condition on the inner boundary $|x| = \varepsilon$, and showed that the corresponding radial minimisers (which are smooth) converge to r_λ as $\varepsilon \rightarrow 0$. This suggests a consistency between the theory in [38] and that based on a straightforward minimisation of I . However, this has not been proved in general, and the limiting case of a domain with infinitely many holes would require a difficult process of homogenisation.

The existence of minimisers of I for W such as (4.6) and arbitrary (non-radial) boundary conditions is an open question. However, Müller & Spector [49] have proved existence when a surface energy term is added to $I(y)$ consisting of a constant multiple of the area of $\partial y(\Omega)$ (a functional related to, but different from, (4.1)).

It is worth contrasting the different effects of a rapid growth of $W(A)$ with A in the theory of cavitation and in that based on (4.1). As we have seen, if W satisfies (4.4) for some $\gamma > 3$ then cavitation is prevented. But for the more realistic model (4.1) rapid growth of W is expected to *promote* fracture for a body under tension, since the body can release a lot of elastic energy by fracturing. By working in a Sobolev space we tacitly assume that the surface energy is infinite, negating this effect. Of course cavitation can presumably occur in the model based on (4.1), but then it has to compete energetically with other types of fracture.

5 Phase Transformations

5.1 A minimisation problem with nonattainment and the formation of microstructure.

To motivate the ideas appearing in this section let us look at the following minimisation problem for the scalar function $u = u(x_1, x_2)$ defined on the square $\Omega = (0, 1) \times (0, 1)$:

$$\text{Min } I(u) = \int_{\Omega} [(u_{x_1}^2 - 1)^2 + u_{x_2}^2] dx_1 dx_2 \quad (5.1)$$

subject to $u(x_1, 0) = 0$.

By constructing a suitable minimising sequence it can be shown that the infimum of I is zero. Roughly speaking one should consider a sequence $\{u^{(j)}\}$ such that the partial derivatives satisfy $u_{x_1}^{(j)} = \pm 1$ and $u_{x_2}^{(j)} = 0$. However in order for the boundary condition to be satisfied a 'transition layer' should exist close to $x_2 = 0$ so that the function matches itself with $u(x_1, 0) = 0$. Putting this in a more precise way consider

$$\bar{u}(x_1, x_2) = \begin{cases} x_1 \phi(x_2) & \text{if } 0 \leq x_1 \leq \frac{1}{2}, \\ (1 - x_1) \phi(x_2) & \text{if } \frac{1}{2} \leq x_1 \leq 1, \end{cases}$$

where $\phi(x_2) = x_2$ if $0 \leq x_2 \leq 1$ and $\phi(x_2) = 1$ if $x_2 \geq 1$. Extending \bar{u} as a one-periodic function of x_1 to $\mathbf{R} \times (0, \infty)$ one can now define

$$u^{(j)}(x_1, x_2) = \frac{1}{j} \bar{u}(jx_1, jx_2).$$

Then $Du^{(j)}(x_1, x_2) = (\bar{u}_{x_1}, \bar{u}_{x_2})(jx_1, jx_2)$ is uniformly bounded and consequently $I(u^{(j)}) \rightarrow 0$ as $j \rightarrow \infty$. However this infimum is *not attained*. If $I(u) = 0$ for some $u \in W^{1,1}$ with $u(x_1, 0) = 0$ then $u_{x_2} = 0$ and hence, integrating in the x_2 direction, $u = 0$. But this implies $I(u) = 1$, a contradiction.

5.2 Young measures

The above problem is a typical example where the infimum of a functional over a class of admissible functions is not attained, and minimising sequences develop a microstructure in which the gradient oscillates more and more finely. The idea of generalised curves or *Young measures* was first introduced and used by L.C. Young to tackle such problems (see his book [69]). In general a Young measure $(\nu_x)_{x \in \Omega}$ is a family of probability measures that gives the limiting distribution of values of a sequence of functions. The following is one possible characterisation [13]. Let $\Omega \subset \mathbf{R}^n$ be an open set. Suppose

$z^{(j)} : \Omega \rightarrow \mathbf{R}^m$ is a sequence of measurable functions. For given x , j and δ define $\nu_{x,\delta}^{(j)}$ to be the probability distribution of the values of $z^{(j)}(p)$ as p is chosen uniformly at random from the ball $B(x; \delta)$. Then

$$\nu_x = \lim_{\delta \rightarrow 0} \lim_{\mu \rightarrow \infty} \nu_{x,\delta}^{(\mu)}$$

with the limit to be understood in the sense of weak* convergence of probability measures. (In general the $z^{(\mu)}$ correspond to a subsequence of the $z^{(j)}$.) For recent surveys of Young measures see [7, 42, 67].

As an example, the reader can check that the Young measure corresponding to the sequence of gradients $u_{x_1}^{(j)}, u_{x_2}^{(j)}$ of any minimising sequence $u^{(j)}$ for the problem (5.1) is given by

$$\nu_x = \frac{1}{2} \delta_{(1,0)} + \frac{1}{2} \delta_{(-1,0)},$$

where $\delta_{(\pm 1,0)}$ denotes the Dirac mass at $(\pm 1, 0)$.

5.3 Microstructure arising from a phase transformation

Now to see what happens in the case of elastic crystals let us look at the problem of a phase transformation in a single crystal of a material, such as the binary alloy Indium-Thallium, where the high temperature phase (*austenite*) has cubic symmetry and the low temperature phase (*martensite*) has tetragonal symmetry. We suppose that θ_c is the temperature at which the phase transformation occurs, and take the reference configuration to be the cubic phase at the temperature $\theta = \theta_c$. We use nonlinear elasticity with free-energy function $W = W(Dy, \theta)$ depending on the temperature. The phase transformation is described by an exchange of stability. Denoting by $K(\theta)$ the set of minimisers of $W(\cdot, \theta)$ in $M^{3 \times 3}$ we assume that

$$\begin{aligned} K(\theta) &= SO(3) && \text{for } \theta > \theta_c, \\ K(\theta) &= \bigcup_{i=1}^3 SO(3)U_i && \text{for } \theta < \theta_c, \\ K(\theta_c) &= SO(3) \cup \bigcup_{i=1}^3 SO(3)U_i, \end{aligned}$$

where

$$\begin{aligned} U_1 &= \text{diag}(\eta_2, \eta_1, \eta_1), \\ U_2 &= \text{diag}(\eta_1, \eta_2, \eta_1), \\ U_3 &= \text{diag}(\eta_1, \eta_1, \eta_2). \end{aligned}$$

The *lattice parameters* η_i in general will depend on temperature. Note that these assumptions are consistent with the frame-indifference and cubic symmetry of W . We call the connected components of $K(\theta)$ *energy wells*; thus,

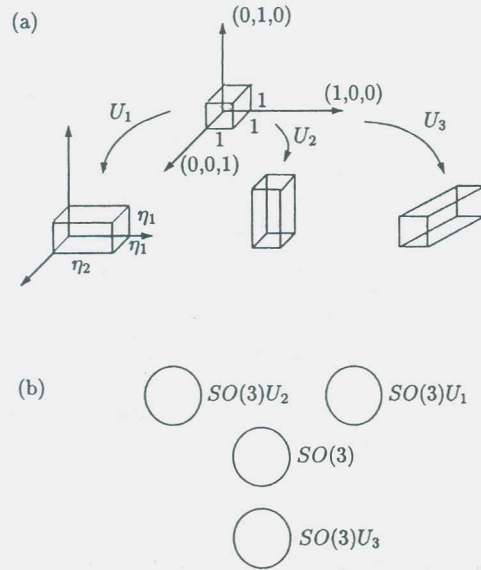


Figure 7: A cubic-to-tetragonal phase transformation. (a) Austenite and the three variants of martensite, (b) the corresponding energy wells $SO(3)$ and $SO(3)U_i$, $i = 1, 2, 3$.

for example, at $\theta = \theta_c$ there is one austenite energy well $SO(3)$ and three martensite energy wells $SO(3)U_i$ corresponding to the three possible variants of martensite. These energy wells are represented schematically by circles in Fig. 7.

By considering different rank-one connections between the different energy wells as explained in Section 3 we can construct different global energy minimisers which are combinations of variants or phases. To illustrate this let us suppose that $\theta = \theta_c$. Then it can be shown [14] that there is no rank-one connection between two matrices on a single well, nor between a martensite well and the austenite well (provided no $\eta_i = 1$, which we assume). However to each matrix on a martensite well there correspond two distinct matrices on each different martensite well. Once we have found such a rank-one connection between martensite wells

$$B - A = a \otimes n,$$

with $A \in SO(3)U_i, B \in SO(3)U_j, i \neq j$, we can construct a corresponding interface and even form a *simple laminate* consisting of the limit as $j \rightarrow \infty$ of a family of layers having normals n , alternating deformation gradients A, B and alternating thicknesses $\lambda/j, (1 - \lambda)/j$ (see Fig. 8).

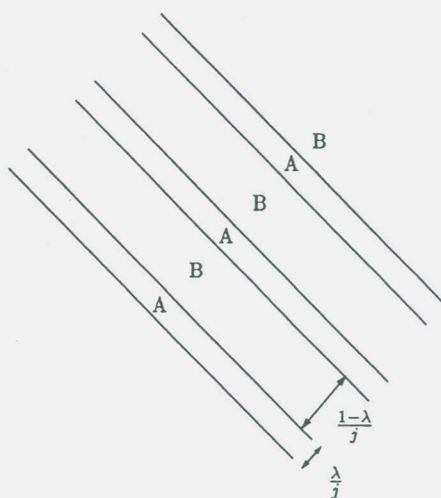


Figure 8: A simple laminate formed using the rank-one connection $B - A = a \otimes n$.

The Young measure corresponding to the sequence $z^{(j)} = Dy^{(j)}$ of deformation gradients generating this microstructure in the limit $j \rightarrow \infty$ is easily verified to be

$$\nu_x = \lambda \delta_A + (1 - \lambda) \delta_B,$$

where δ_A denotes the Dirac mass at A .

As another example we can consider a *double laminate* shown in Fig. 9 formed from four matrices A, B, C, D on martensite wells with rank-one connections

$$\begin{aligned} A - B &= a \otimes n, \\ C - D &= b \otimes m, \\ (B + \mu a \otimes n) - (D + \lambda b \otimes m) &= c \otimes l, \end{aligned}$$

and having the Young measure

$$\nu_x = \sigma(\mu \delta_A + (1 - \mu) \delta_B) + (1 - \sigma)(\lambda \delta_C + (1 - \lambda) \delta_D).$$

Note that since, for example, $\text{rank}(A - C) > 1$ in general, transition regions are required to interpolate between the single laminates, as in problem (5.1). The volume of these layers tends to zero as $j \rightarrow \infty$ and so the energy contribution due to the deformation gradients not belonging to $K(\theta_c)$ vanishes in the limit.

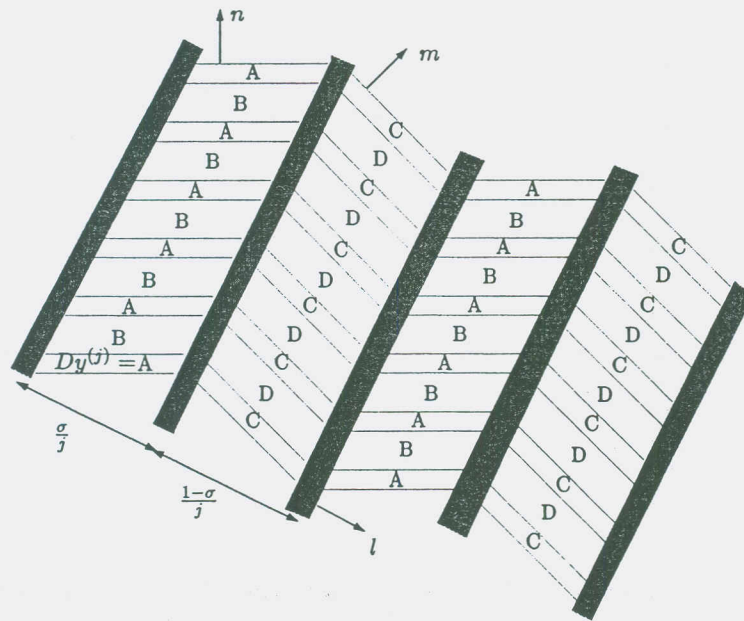


Figure 9: A double laminate formed from four matrices on martensite wells, showing the values of the deformation gradient $Dy^{(j)}$. The layers in which $Dy^{(j)}$ takes the values A, B, C, D have thicknesses $\frac{\mu}{j^2}$, $\frac{(1-\mu)}{j^2}$, $\frac{\lambda}{j^2}$, $\frac{(1-\lambda)}{j^2}$ respectively. The shaded areas are transition regions whose thicknesses are $O\left(\frac{1}{j^2}\right)$.

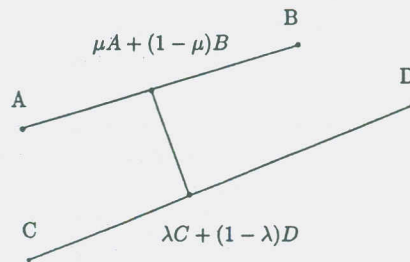


Figure 10: Diagram showing the rank-one connections in the double laminate shown in Fig. 9; each line represents a rank-one connection.

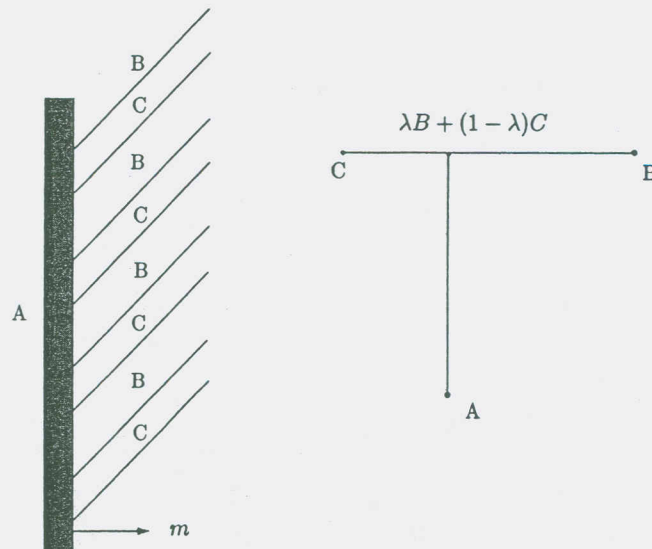


Figure 11: The austenite-martensite interface, and the corresponding rank-one connections. The matrix A is on the austenite well, B and C on different martensite wells. The corresponding Young measure is given by $\nu_x = \delta_A$ if $x \cdot m < \alpha$, and by $\nu_x = \lambda\delta_B + (1 - \lambda)\delta_C$ if $x \cdot m > \alpha$.

It is sometimes more convenient to show the different rank-one connections involved in a microstructure using a diagram such as Fig. 10 in which they are indicated by straight lines.

In general different sorts of microstructure involving laminates can be analysed by solving the algebraic problem of finding matrices on the energy-wells having the appropriate rank-one connections. Interesting examples are the *austenite-martensite interface*, in which a single laminate of martensite is connected along a planar interface to an austenite region (see Fig. 11 and [14]), and the *wedge* [22].

Clearly an important question for the analysis of microstructures is to classify the Young measures arising from sequences of gradients. Important necessary conditions are the *minors relations*. In general a minor $J = J(A)$ is a subdeterminant of an $m \times n$ matrix A . For example, in the case $m = n = 3$ there are 19 such minors in all, given by the elements of A , $\text{cof } A$ and $\det A$. If $J : M^{m \times n} \rightarrow \mathbf{R}$ is a minor and $(\nu_x)_{x \in \Omega}$ is the Young measure corresponding to a sequence $Dy^{(j)}$ of gradients satisfying suitable bounds (e.g. uniformly bounded in L^∞) then

$$J \left(\int_{M^{m \times n}} A d\nu_x(A) \right) = \int_{M^{m \times n}} J(A) d\nu_x(A) \quad \text{a.e. } x \in \Omega.$$

In particular for $m = n = 3$

$$\begin{aligned} Dy(x) &= \int_{M^{3 \times 3}} A d\nu_x(A), \\ \text{cof } Dy(x) &= \int_{M^{3 \times 3}} \text{cof } A d\nu_x(A), \\ \det Dy(x) &= \int_{M^{3 \times 3}} \det A d\nu_x(A), \end{aligned}$$

where y denotes the weak limit of $y^{(j)}$. The minors relations are not sufficient for a parametrised measure $(\nu_x)_{x \in \Omega}$ to be a Young measure of gradients (c.f. [15, 23]). Necessary and sufficient conditions in terms of quasiconvexity have been obtained by Kinderlehrer & Pedregal [41], but on account of our lack of understanding of quasiconvexity these conditions are at present more of theoretical interest than a practical tool.

5.4 The two-well problem

It is impossible to adequately survey here the very active field of the analysis of crystal microstructure, and the reader should consult the cited references. In this section we consider briefly one special problem in which the issue of nonattainment of a minimum has been at least partially clarified. This is the *two-well problem* arising, for example, in orthorhombic to monoclinic transformations, in which $K = K(\theta)$ has the form

$$K = SO(3)U_1 \cup SO(3)U_2$$

for distinct positive definite symmetric matrices U_1, U_2 . We suppose that the minimum value of $W(\cdot, \theta)$, attained on K , is zero. The case when $\det U_1 = \det U_2$ is discussed in [15], where it is shown that via a change of variables one can represent the above set K in the form

$$K = SO(3)S^+ \cup SO(3)S^-,$$

with $S^\pm = 1 \pm \delta e_3 \otimes e_1$, $\delta > 0$ and $\{e_1, e_2, e_3\}$ an orthonormal basis for \mathbf{R}^3 . Consider the problem of minimising

$$I(y) = \int_{\Omega} W(Dy, \theta) dx$$

subject to the linear boundary conditions

$$y|_{\partial\Omega} = Fx,$$

where $F \in M_+^{3 \times 3}$. It is proved in [15] that the infimum of I is zero (i.e. there is a zero energy microstructure) if and only if $C = F^T F \in \mathcal{R}$, where \mathcal{R} consists of symmetric matrices of the form

$$\begin{bmatrix} C_{11} & 0 & C_{13} \\ 0 & 1 & 0 \\ C_{13} & 0 & C_{33} \end{bmatrix}$$

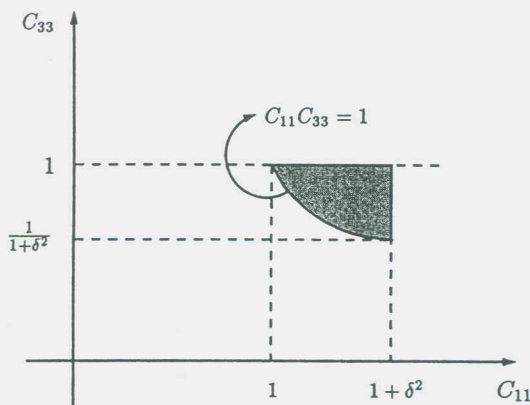


Figure 12: The set of strains C corresponding to zero-energy microstructures in the two-well problem; (C_{11}, C_{33}) must belong to the shaded region and $C_{13}^2 = C_{11}C_{33} - 1$.

with (C_{11}, C_{33}) in the region shown in Fig. 12 defined by the inequalities $C_{11} \leq 1 + \delta^2$, $C_{33} \leq 1$ and $C_{11}C_{33} \geq 1$, and with $C_{13}^2 = C_{11}C_{33} - 1$.

If $C \in \mathcal{R}$ satisfies either $C_{11} = 1 + \delta^2$, or $C_{33} = 1$ then F has the form

$$F = \lambda A + (1 - \lambda)B,$$

with $A \in SO(3)S^+$, $B \in SO(3)S^-$, $\lambda \in [0, 1]$, and the Young measure corresponding to the sequence $Dy^{(j)}$ for any minimising sequence $y^{(j)}$ is given by

$$\nu_x = \lambda \delta_A + (1 - \lambda) \delta_B.$$

In particular, if $\lambda \neq 0, 1$ (i.e. if $F \notin K$) then the Young measure is not a Dirac mass and so the *minimum is not attained*. Recent work of Müller and Šverák [50] suggests that, surprisingly, the minimum may be attained if C takes other values in \mathcal{R} , though by a very irregular deformation.

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