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Analysis of Microstructures and Phase Transition Phenomena in One-Dimensional, Non-Linear Elasticity by Convex Optimization

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Abstract We propose a general method to determine the theoretical microstructure in one dimensional elastic bars whose internal deformation energy is given by non-convex polynomials. We use non-convex variational principles and Young measure theory to describe the optimal energetic configuration of the body. By using convex analysis and classical characterizations of algebraic moments, we can formulate the problem as a convex optimal control problem. Therefore, we can estimate the microstructure of several models by using non-linear programming techniques. This method can determine the minimizers or the minimizing sequences of non-convex, variational problems used in one-dimensional, non-linear elasticity.

Keywords alloys microstructure · Young measures theory · non-convex variational principles · moments problems · non-linear elasticity

1 Introduction

In this paper we deal with the mathematical analysis and the numerical solution of variational principles that describe the total energy of one-dimensional, elastic bodies. The general form of these problems is given by the following formulation:

$$\begin{array}{ll}\min\limits_{u} & \int_0^1 \left\{\phi\left(x,u'\right)+\psi\left(x,u\right)\right\} dx \\ \text{s.t.} & u' \geq 0 \\ & u(0)=0,\ u(1)=\alpha\end{array} \qquad (1)$$

where the admissible function $u : [0,1] \to \mathbb{R}$ stands for the displacement of every point $x \in [0,1]$ on a particular one-dimensional body settled in the interval $[0,1]$. Hence, u' accounts for the unitary deformation along the body. The functions ϕ and ψ stand respectively for the potential of internal deformation energy and the potential energy of external forces. These energy potentials may vary with the dimension x of the body. The positivity of the derivative u' comes from the fact that we can not expect negative deformations. The parameters of the problem are the length of the body and the imposed elongations at the edges of the body. Without loss of generality we choose them as 1 for the whole length; 0 for the first boundary condition and α for the second boundary condition. For an introduction to variational models in elasticity see references (Antman 2004; Cherkaev 2000; James 1979; Müller 1990, 1998; Pedregal 2000; Truskinovsky and Zanzotto 1995, 1996). In order to determine the existence of minimizers of the variational problem (1), we select the Sobolev space $H_0^{1,p} + g_0$, where p depends on the particular potential ϕ and g_0 comes from the particular boundary conditions of the problem. In our case we should take $g_0(x) = \alpha x$.

In this work we will carry out the analysis of general models in the form (1), where the non-convex dependence of ϕ in u' can be described by a polynomial expression like:

$$\phi(x,\lambda) = \sum_{k=0}^{K} c_k(x)\lambda^k, \quad c_K > 0, \quad K > 1. \qquad (2)$$

To attain this goal we will use the corresponding generalized formulation of (1) in Young measures and their corresponding representation as algebraic moments by following the method of moments for non-convex variational problems. This method has been proposed in (Egozcue et al 2001, 2003; Meziat 2001). A more theoretical approach with applications to optimal design can be seen in (Bonnetier and Conca 1994). See (Aubert and Tahraoui 1996; Balder 1995; Kinderlehrer and Pedregal 1991, 1994; Pedregal 1997, 2000; Roubicek 1997; Young 1980) for an introduction to the theory of Young measures and its implications in non-convex variational problems and non-linear, optimal design problems. Many

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other researchers have proposed alternative ways to solve generalized problems in Young measures. However, they do not consider the restrictions on the derivative of (1). As instance see (Bartels and Roubicek 2004; Bonnetier and Conca 1994; Carstensen and Plechac 1997; Carstensen and Roubícek 2000; Muñoz and Pedregal 2000; Nicolaides and Walkington 1992; Pedregal 1995, 1996; Roubicek 1996).

The more important feature of the method proposed here is its ability to analyse non-convex variational problems with constraints on the derivative like (1). In spite of the limitation of the method to analyse cases in higher dimensions, our approach works well in many interesting models in one-dimensional, non-linear elasticity and it is useful to face open questions in materials science.

This paper is organized as follows: in Section 2 we will present the analysis of the problem (1) by using standard techniques of Young measures and the classical Stieltjes Truncated Moment Problem which is well suited to treat the constraints into the derivative given in (1). In Section 3 we solve several examples by using proper computational tools from non-linear mathematical programming. In Section 4 we present our results to the light of physical concepts like elasticity theory, stable energy states of crystalline lattices, solid phases and the development of microstructures in one-dimensional, non-linear, elastic bodies. In the Appendix we present the theory of the method by following previous ideas on the theory of the method of moments stated in (Egozcue et al 2001, 2003; Meziat 2001).

2 Analysis of the Problem by Using the Moments of Young Measures

To analyze the variational problem (1), we state it in the following form:

$$\begin{aligned} &\min_u \int_0^1 \{\Phi(x,u'(x)) + \psi(x,u(x))\}\, dx \\ &\text{s.t. } u(0)=0,\ u(1)=\alpha \end{aligned} \tag{3}$$

where Φ is defined as:

$$\Phi(x,\lambda) = \begin{cases} \phi(x,\lambda) & \text{when } \lambda \geq 0 \\ \infty & \text{otherwise} \end{cases} \tag{4}$$

and the admissible functions u are supposed to belong to the Sobolev space $H_0^{1,p} + g_0$. Here $p \leq K$ as imposed by the growth of the polynomial ϕ. In this formulation we can apply Young measures theory for non-convex variational problems (Pedregal 1997). Thus, we can transform problem (3) into a new generalized problem defined in sets of parametrized measures as:

$$\begin{aligned} &\min_v \int_0^1 \left\{\int_R \Phi(x,\lambda)\, d\mu_x(\lambda) + \psi(x,u)\right\} dx \\ &\text{s.t. } u'(x) = \int_R \lambda\, d\mu_x(\lambda) \text{ for every } x \in [0,1] \\ &\qquad u(0)=0,\ u(1)=\alpha \end{aligned} \tag{5}$$

where every measure μ_x is a probability distribution supported in the real line R. The theory of Young measures claims that every generalized problem (5) always has a minimizer, even if the original variational problem (3) does not have any, see (Pedregal 1997). Moreover, the generalized formulation (5) is a relaxation of (3) as they share the same infimum value. Young measure solutions of the generalized principle (5) provide information about the existence of minimizers of the variational problem (3) and the general behavior of its minimizing sequences. Readers can see a good account on this theory in the current literature: (Pedregal 1997) and (Roubicek 1997).

According to the definition of the function Φ in (4), we can formulate (5) as

$$\begin{aligned} &\min_v \int_0^1 \left\{\int_0^\infty \phi(x,\lambda)\, d\mu_x(\lambda) + \psi(x,u)\right\} dx \\ &\text{s.t.} \\ &\text{support}(\mu_x) \subset [0,\infty), \quad u'(x) = \int_0^\infty \lambda\, d\mu_x(\lambda) \\ &\text{for every } x \in [0,1] \quad \text{with} \quad u(0)=0,\ u(1)=\alpha \end{aligned} \tag{6}$$

and we can use the polynomial form of ϕ given in (2) in order to transform (6) into the following optimization problem:

$$\begin{aligned} &\min_{\mathbf{m}} \int_0^1 \left\{\sum_{k=0}^K c_k(x) m_k(x) + \psi(x,u)\right\} dx \\ &\text{s.t. } u'(x) = m_1(x) \quad \text{for every } x \in [0,1] \\ &\qquad u(0)=0,\ u(1)=\alpha \end{aligned} \tag{7}$$

where the new control variable $\mathbf{m} \in \mathbb{R}^{K+1}$ must belong to the convex set M of vectors in $\mathbb{R}^{K+1}$ whose entries are the algebraic moments of a probability measure supported in $[0,\infty)$. In order to characterize the variable $\mathbf{m}$ as a vector of moments, we use the solution of the classical Stieltjes Truncated Moment Problem (Akhiezer 1962; Curto and Fialkow 1991; Karlin 1966; Krein 1977; Shohat and Tamarkin 1943). By using this classical result, we can define (7) as the following optimal control problem constrained by matrix inequalities:

$$\begin{aligned} &\min_{\mathbf{m}} \int_0^1 \left\{\sum_{k=0}^K c_k(x) m_k(x) + \psi(x,u)\right\} dx \\ &\text{s.t. } u(0)=0,\ u(1)=\alpha, \\ &\qquad u'(x) = m_1(x), \\ &\qquad H_1(x) = (m_{i+j}(x))_{i,j=0}^{\frac{K}{2}} \geq 0, \\ &\qquad H_2(x) = (m_{i+j+1}(x))_{i,j=0}^{\frac{K}{2}-1} \geq 0 \\ &\text{and } m_0(x)=1 \text{ for every } x \in [0,1] \quad \text{when } K \text{ is even.} \end{aligned} \tag{8}$$

Analogous expressions hold when K is odd by using the Hankel forms:

$$H_3 = (m_{i+j})_{i,j=0}^{\frac{K-1}{2}} \quad \textit{and} \quad H_4 = (m_{i+j+1})_{i,j=0}^{\frac{K-1}{2}} \tag{9}$$

instead of H_1 and H_2 Hankel forms in (8). Herein the reader should notice that all the ensuing results are valid for odd K just by putting the forms H_3 and H_4 into the places of the Hankel forms H_1 and H_2.

The essential feature of the optimal control problem (8) is its convex structure in the control variable $\mathbf{m}$. This fact implies existence of minimizers. See (Fattorini 1999; Milyutin and Osmolovskii 1998; Mordukhovich 1998; Muñoz and Pedregal 2000). Moreover, its particular convex form

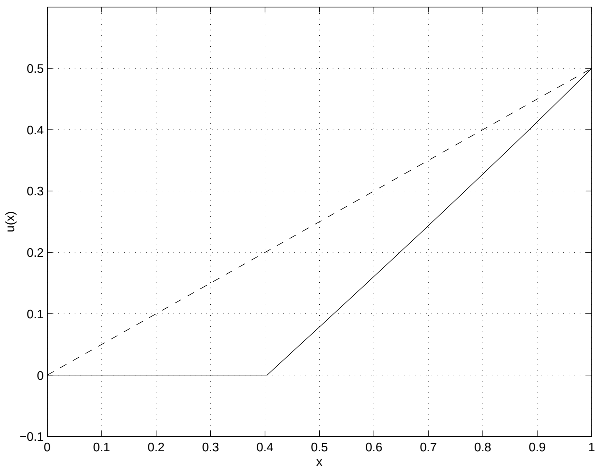

Fig. 1 Estimated minimizer for problem (13).

is well suited to algorithms and software for non-linear, convex mathematical programs. See (Bazaraa et al 1993; Ben-Tal and Nemirovski 2001; Castillo et al 2001; Hoang 1997; Nesterov and Nemirovskii 1995; Pedregal 2003; Renegar 2001). In the following section we will exploit this fact when we present the numerical treatment of these problems as a big convex mathematical program.

A remarkable feature of this approach is its ability to cope with particular constraints on the derivative of the admissible functions, i.e. $u' \geq 0$, avoiding new complexities into the analysis of the problem. This is true because we can characterize sets of moments of probability measures supported in intervals by matrix inequalities, exactly in the same way that we do for the entire real line. As instance consider the Stieltjes Truncated Moment Problem used here for probabilities supported in the semi-axis $u' \geq 0$.

3 Practical Solution by Using Non Linear Programming

In this section we show how determine both: minimizers and minimizing sequences of (1). A detailed explanation of these possibilities follows. When

$$\mu_x^* = \delta_{s(x)} \quad \text{for every } x \in [0,1] \tag{10}$$

the integration procedure

$$u^*(x) = \int_0^x s(r)\,dr \tag{11}$$

defines a minimizer for (1) in the Sobolev space $H_0^{1,p}+g_0$. However, when there exist optimal parametrized measures supported in two points, i.e.:

$$\mu_x^* = p_1(x)\delta_{s_1(x)} + p_2(x)\delta_{s_2(x)} \text{ for every } x \in I \subset [0,1] \tag{12}$$

where I is a subinterval of $[0,1]$, $p_1(x)+p_2(x) = 1$ and $p_1(x)$, $p_2(x) > 0$ for every $x \in I$, the problem (1) may lack of minimizers. Nevertheless, we can use the information enclosed in every parametrized measure in (12) to determine how an admissible function can decrease the value of the functional in (1). We must carry out a step-wise integration procedure by taking the slope of the function from the values $s_1(x)$ and $s_2(x)$ according to their respective probabilities: $p_1(x)$ and $p_2(x)$. Thus, we obtain a sort of saw-tooth like graph on the interval I. See (Chipot 1991; Chipot and Kinderlehrer 1988; Chipot et al 1995; Pedregal 1997, 2000). To estimate every parametrized measure μ_x^* we solve the optimal control problem (8) by using a discrete model and standard routines for non-linear programming via the AMPL modelling language (Fourer et al 2002) and non-linear programming algorithms like active-set type and trust regions as described in (Bazaraa et al 1993; Castillo et al 2001; Conn et al 2000; More and Wright 1993).

i	m_1	m_2	m_3	m_4	optimal measure
1 . . . 20	0.000	0.000	0.000	0.000	$\delta_{0.000}$
21. . . 50	0.833	0.693	0.577	0.481	$\delta_{0.833}$

Table 1 Optimal moments and optimal parametrized measures for problem 13.

3.1 Example 1

Consider the variational problem:

$$\begin{aligned} &\min_u \int_0^1 \left\{ \left(1-u'(x)^2\right)^2 + u(x)^2 \right\} dx \\ &\text{s.t.} \quad u(0)=0, \quad u(1)=\tfrac{1}{2} \\ &\qquad u'(x) \geq 0 \quad \text{for every } x \in [0,1] \end{aligned} \tag{13}$$

which is transformed into the optimal control problem:

$$\begin{aligned} &\min_{\mathbf{m}} \int_0^1 \left\{ (1-2m_2(x)+m_4(x)+u(x)^2 \right\} dx \\ &\text{s.t.} \quad u'(x) = m_1(x), \\ &\qquad \begin{pmatrix} 1 & m_1(x) & m_2(x) \\ m_1(x) & m_2(x) & m_3(x) \\ m_2(x) & m_3(x) & m_4(x) \end{pmatrix} \geq 0 \quad \text{and} \\ &\qquad \begin{pmatrix} m_1(x) & m_2(x) \\ m_2(x) & m_3(x) \end{pmatrix} \geq 0 \\ &\qquad \text{for every } x \in (0,1) \\ &\text{with } u(0)=0, \quad u(1)=\tfrac{1}{2}. \end{aligned} \tag{14}$$

This optimization problem can be formulated as the following convex mathematical program:

$$
\begin{aligned}
\min_{\mathbf{m}} \;\; & \Delta \sum_{i=1}^{N} \left(1 - 2m_2(x_i) + m_4(x_i) \right. \\
& \left. + \left(\Delta \sum_{j=1}^{i} m_1(x_j) \right)^2 \right) \\
s.t. \;\; & \sum_{i=1}^{N} m_1(x_i) = \frac{u(1)-u(0)}{\Delta} = \frac{1}{2\Delta} \\
& \begin{pmatrix} 1 & m_1(x_i) & m_2(x_i) \\ m_1(x_i) & m_2(x_i) & m_3(x_i) \\ m_2(x_i) & m_3(x_i) & m_4(x_i) \end{pmatrix} \geq 0 \quad and \\
& \begin{pmatrix} m_1(x_i) & m_2(x_i) \\ m_2(x_i) & m_3(x_i) \end{pmatrix} \geq 0 \quad \text{for every } i = 1, \ldots, N \\
\text{with } & \Delta = \frac{1}{N},
\end{aligned} \tag{15}
$$

where the points $x_i = \frac{i}{N}$ for $i = 1, \ldots, N$ define a discrete net of N points on the interval $[0, 1]$.

By using non-linear programming, we obtain the optimal values $\mathbf{m}^*(x_i)$ on a particular discrete net of 50 points x_i evenly distributed along the interval $[0, 1]$. See results in Table 1. Next, we recover every parametrized measure $\mu^*_{x_i}$ from their algebraic moments 1, $m_1^*(x_i)$, $m_2^*(x_i)$, $m_3^*(x_i)$, $m_4^*(x_i)$. In Figure 1 we simulate the behavior of a minimizing sequence. It is very important to notice here that this figure has been constructed by using the results obtained from the numerical computation and the procedure described above. Thus, we can postulate that problem (13) might have a minimizer like:

$$
u^*(x) = \begin{cases} 0 & \text{when} \quad 0 \leq x \leq 0.4 \\ 0.833(x - 0.4) & \text{when } 0.4 \leq x \leq 1. \end{cases} \tag{16}
$$

Although we could use other methods for non-linear, non-convex mathematical programs in the formulation (1), we would succeed only in those cases which admit minimizers. But this condition can not be certified a priori in general cases fitting (1). Thus, we point out an important virtue of the method of moments proposed in this work: it works well in arbitrary, non-convex, variational problems (1) whether they have or they have not minimizers.

3.2 Example 2

Here we focus on the non-convex variational problem

$$
\begin{aligned}
& \min_u \int_0^1 \left\{ f\left(u'(x)\right) + u(x)^2 \right\} dx \\
& \text{s.t.} \quad u(0) = 0, \quad u(1) = \tfrac{1}{2} \\
& \qquad\; u'(x) \geq 0 \quad \text{for every } x \in [0, 1]
\end{aligned} \tag{17}
$$

where the potential f is given by the following non-convex, four degree polynomial:

$$
f(x) = x^4 - 3x^3 - 5x^2 + 7x. \tag{18}
$$

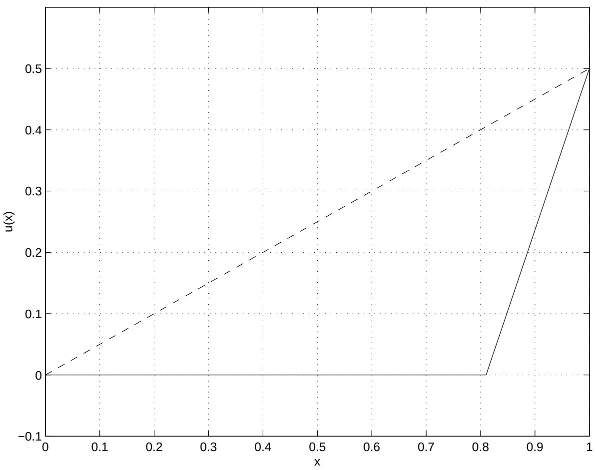

Fig. 2 Estimated minimizer for problem (17) with the potential (18).

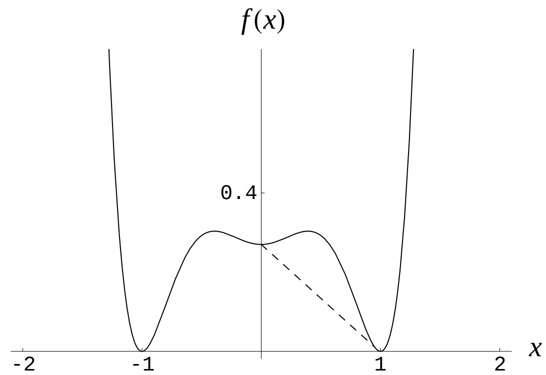

Fig. 3 Plot of the 6$^{\text{th}}$ degree polynomial described by eq: (21). The doted line is its convex envelope in $[0, \infty)$.

By solving the corresponding convex mathematical program on a net of 50 points, we obtain the following optimal parametrized measures:

$$
\begin{aligned}
\mu^*_{x_i} &= \delta_0 \quad\;\; for \quad i = 1, ..., 41 \\
\mu^*_{x_i} &= \delta_{2.78} \; for \quad i = 42, ..., 50
\end{aligned} \tag{19}
$$

and herein the minimizer shown in Figure 2. From these results we infer the existence of a minimizer like:

$$
u^*(x) = \begin{cases} 0 & \text{when} \quad 0 \leq x \leq 0.82 \\ 2.78(x - 0.82) & \text{when } 0.82 \leq x \leq 1. \end{cases} \tag{20}
$$

3.3 Example 3

We solve here the variational problem (17) where f is the non-convex, sixth degree polynomial

$$
f(x) = x^6 - \frac{173}{100}x^4 + \frac{23}{50}x^2 + \frac{27}{100} \tag{21}
$$

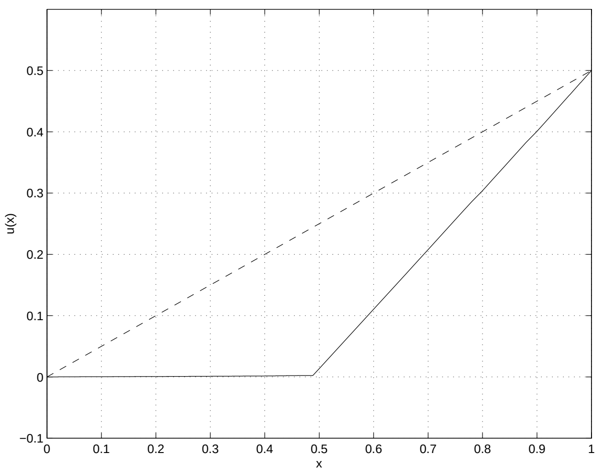

Fig. 4 Estimated minimizer for problem (17) with the potential (21).

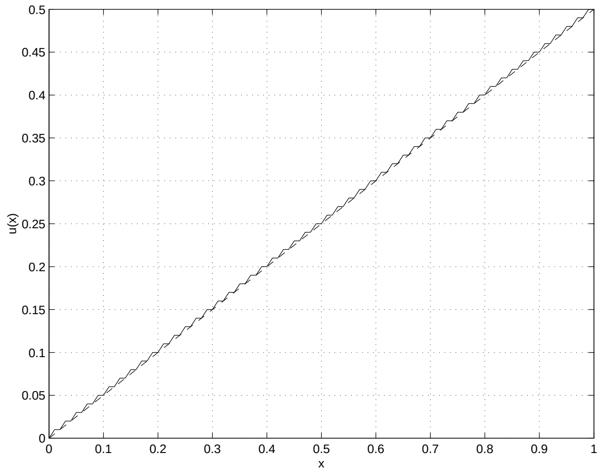

Fig. 5 Minimizing sequence for problem (25), the dashed line is $u(x) = \frac{1}{2}x$.

which is shown in Figure 3 beside its convex envelope on the semi-axis $[0, \infty)$. The discrete model for this problem is the following convex program:

$$\begin{array}{ll}\min_{\mathbf{m}} \Delta \sum_{i=1}^{N} \Bigg(\frac{27}{100} + \frac{23}{50} m_2(x_i) - \frac{173}{100} m_4(x_i) \\ \quad + m_6(x_i) + \left(\Delta \sum_{j=1}^{i} m_1(x_j) \right)^2 \Bigg) \\ \text{s.t.} \ \sum_{i=1}^{N} m_1(x_i) = \frac{u(1)-u(0)}{\Delta} = \frac{1}{2\Delta} \\ \quad \begin{pmatrix} m_1(x_i) & m_2(x_i) & m_3(x_i) \\ m_2(x_i) & m_3(x_i) & m_4(x_i) \\ m_3(x_i) & m_4(x_i) & m_5(x_i) \end{pmatrix} \geq 0 \quad and \\ \quad \begin{pmatrix} 1 & m_1(x_i) & m_2(x_i) & m_3(x_i) \\ m_1(x_i) & m_2(x_i) & m_3(x_i) & m_4(x_i) \\ m_2(x_i) & m_3(x_i) & m_4(x_i) & m_5(x_i) \\ m_3(x_i) & m_4(x_i) & m_5(x_i) & m_6(x_i) \end{pmatrix} \geq 0 \\ \quad \text{for every } i = 1, \ldots, N. \end{array} \tag{22}$$

By taking a mesh of $N = 50$ points, we obtain the optimal parametrized measures:

$$\begin{array}{ll} \mu^*_{x_i} = \delta_0 & for \quad i = 1, ..., 24 \\ \mu^*_{x_i} = \delta_{0.97} & for \quad i = 25, ..., 50 \end{array} \tag{23}$$

which provide the minimizer shown in Figure 4 and suggest the existence of a minimizer with the form:

$$u^*(x) = \begin{cases} 0 & \text{when} \quad 0 \leq x \leq 0.485 \\ 0.97(x - 0.485) & \text{when } 0.485 \leq x \leq 1. \end{cases} \tag{24}$$

The following example shows that we can not always expect existence of minimizers for non-convex variational problems given in the general form (1).

3.4 Example 4

In this example we face the same kind of non-convex, variational problem as we did in the previous example, but we change slightly the external forces potential ψ. Thus, we consider:

$$\begin{array}{ll} \min_u \int_0^1 \left\{ f\left(u'(x)\right) + \left(u(x) - \frac{1}{2}x\right)^2 \right\} dx \\ \text{s.t.} \quad u(0) = 0, \quad u(1) = \frac{1}{2} \\ \quad\quad u'(x) \geq 0 \quad \text{for every } x \in [0, 1] \end{array} \tag{25}$$

where the function f is the sixth degree, non-convex polynomial given in (21). By solving the corresponding convex mathematical program over a discrete net of 50 points we obtain the following optimal Young measure solution:

$$\mu^*_{x_i} = 0.484\delta_0 + 0.516\delta_{0.97} \quad \text{for every } i = 1, ..., 50 \tag{26}$$

which entails oscillatory minimizing sequences like the one shown in Figure (5). Since the optimal parametrized measures are supported in two points all along the interval $[0, 1]$, the variational problem (25) lacks of minimizers in the Sobolev space $H^{1,6}_0 + g_0$. In this case the oscillatory behavior is promoted by the alternation between two slopes: 0 and 0.97, which are preferred according to the corresponding proportions 48.4% and 51.6% all along the interval $[0, 1]$. The finer the size scale in which this oscillation takes place, the lesser the value of the functional in (25). This situation is illustrated in Figure 5.

At this point the reader should understand the different possibilities for non-convex variational problems given in the general form (1): existence of minimizers, lacking of minimizers and different kinds of oscillatory behavior related to the non-convex form of the integrand in (1). The approach presented in this work offers an interesting frame for analyzing and understanding non-linear phenomena present in one-dimensional, non-linear elastic bodies. We discuss this subject in the following section.

4 Physical implications and conclusions

The non-linear elastic behavior of several materials has very important implications in engineering and design, for example consider the typical strain-stress graph for low-carbon steels given in Figure 6 and the associated deformation energy potential in Figure 7. Since the stress in Figure 6 can be identified with the derivative $\frac{\partial \phi}{\partial \epsilon}$, then it is clear that the deformation energy potential ϕ does not have a convex dependence on the deformation u' when we consider materials with a non-linear, elastic behavior. In this situation we can not apply neither the Direct Method of the Calculus of Variations (Buttazzo and Giaquinta 1998; Cesari 1983; Dacorogna 1989; Ekeland and Temam 1999; Giaquinta 1996; Jost et al 1999; Ashby 1996; Cherkaev 2000; Hibbeler 1994; Ruoff 1973; Shackelford 1996) nor computational techniques of Mathematical Programming (Castillo et al 2001; More and Wright 1993) because they do not work well when the potential ϕ lacks of convexity in the deformation variable $\epsilon = u'$. See (Ball 1977; Ekeland 1979; Mascolo and Schianchi 1983; Mordukhovich 1998; Muñoz and Pedregal 1998, 2000; Ornelas 2003; Pedregal 1997, 2000; Roubicek 1997; Young 1942, 1980) for a review of the implications of convexity in the existence of minimizers of variational and optimal design problems.

From a physical point of view, the mechanical behavior of a body, when stressed further than the elastic limit of the material, is a complex phenomenon involving geometrical and physical properties of the atoms conforming its crystalline lattice. When the material is charged to such high stresses, it may take one between two kinds of crystalline arrangements which correspond to two energetically stable configurations of the atoms of the material. This microscopic transformation is reflected in the size, kind and number of clusters in which the different solid phases grow up inside the material; beside that, we must consider some important macroscopic phenomena like material fluence, hardening and finally cracking and rupture. See (Ashby 1996; Ericksen 1980; Hibbeler 1994; Ruoff 1973; Shackelford 1996; Valencia 1998) for a description of the physical changes of engineering materials subject to different load conditions. See (Antman 2004; Ball and James 1987, 1992; Battacharya 1991; Battacharya et al 1997; Bauman and Phillips 1990; Ericksen 1980, 1986; Fonseca 1985; Fonseca et al 1994; Friesecke 1994; James 1979; Kinderlehrer 1988; Kohn and Müller 1992, 1994; Lurie 1990; Müller 1990, 1997; Truskinovsky and Zanzotto 1995; Otto and Kohn 1997) for a better description of non-convex, variational principles as models for the mechanical and physical behavior of materials in non-linear elasticity.

It is not our aim in this work to address the physical nature of these processes. However, we strongly emphasize that the mathematical and computational analysis that we propose here for treating the variational problem stated in (1), do provide important elements about the energetic configuration of the body when we are studying non-linear, elastic models. In short, we can determine the internal microstructure of the material.

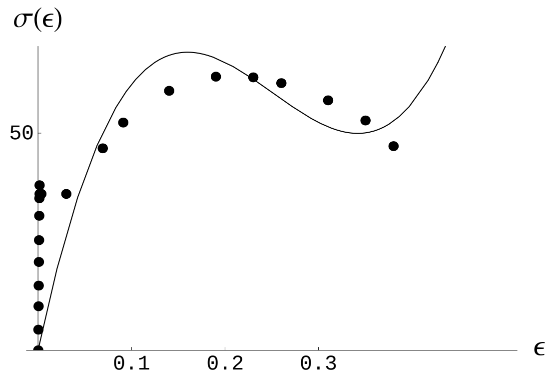

Fig. 6 Solid line is the third degree polynomial fit of one stress-strain curve for commercial steels. Experimental measurements (shown here as discrete dots) have been taken from (Hibbeler 1994).

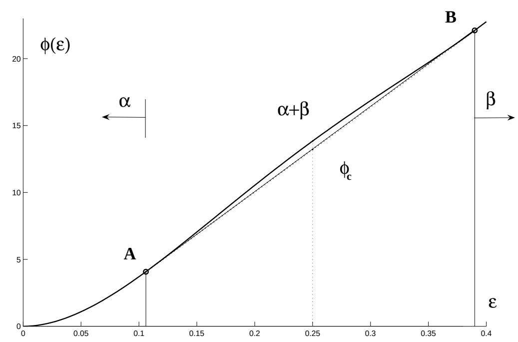

Fig. 7 Deformation energy potential (31) and its convex envelope.

It has been recently proposed that Young measure analysis is a good setting to study non-linear phenomena such as the formation of microstructures in industrial materials like low carbon steels for instance. See (Carstensen and Plechac 1997; Carstensen and Roubícek 2000; Luskin 1996; Matos 1992; Müller 1997, 1998; Nicolaides and Walkington 1992; Nicolaides et al 1995; Pedregal 1997, 2000; Roubicek 1995, 1996) for recent accounts on the role of Young measures in non-linear elasticity and materials science. See (Ashby 1996; Ball and James 1987, 1992; Ericksen 1980, 1986; James 1979; Kohn and Müller 1992, 1994; Luskin 1996; Müller 1990; Otto and Kohn 1997; Shackelford 1996; Truskinovsky and Zanzotto 1995; Valencia 1998) for a comprehensive treatment of the physical features of microstructure in engineering materials. We will use the method of moments for calculating Young measure solutions of non-convex variational problems used as models in non-linear elasticity. The essentials of this application and some examples follow.

4.1 Convex envelopes and stable energetic configurations

Let us focus on the non-convex nature of the deformation energy potential ϕ and its convex envelope ϕ_c shown in Figure 7. If we select a particular deformation amount ϵ located between the points A and B, the convex envelope ϕ_c attains a lower energetic level for the same deformation, that is

$$\phi_c(\epsilon) < \phi(\epsilon) \quad \text{for } \epsilon \in (A_x, B_x) = (0.106, 0.390). \tag{27}$$

From a geometric point of view, we observe that the point $(\epsilon, \phi_c(\epsilon))$ on the graph of ϕ_c can be described as a convex combination of the points A and B on the graph of the function ϕ. That is

$$\begin{aligned}(\epsilon, \phi_c(\epsilon)) &= p_1 (\epsilon_1, \phi(\epsilon_1)) + p_2 (\epsilon_2, \phi(\epsilon_2)) \\ &= p_1 A + p_2 B\end{aligned} \tag{28}$$

where p_1 and p_2 define a convex combination (i.e., $p_1, p_2 > 0$ and $p_1 + p_2 = 1$). This geometric information can be turned into a very deep physical observation, which has also been noticed previously by other authors (Ball and James 1987, 1992; Carstensen and Roubícek 2000; James 1979; Müller 1990, 1997, 1998).

1. As the body tries to minimize the overall potential deformation energy ϕ, it prefers a combination of the energy states A and B instead of the higher energetic value $\phi(\epsilon)$.
2. The convex combination (28) gives the proportions in which the energy states A and B should be mixed to produce the lowest energy value ϕ_c while still producing the deformation ϵ.

Several design materials, as low carbon steels for example, may exhibit two solid phases related to different stable energetic configurations in their crystalline net. As instance, consider the Body Cubic Centered (BCC) and Face Centered Cubic (FCC) solid phases in commercial steels (Ashby 1996; Hibbeler 1994; Shackelford 1996). The way in which these solid phases spread along the body has a strong influence into the mechanical properties of the material. Hence, we should determine the way in which two different solid phases spread and mix along the body to form a particular *microstructure* according to the external charges acting upon the body. See (Müller 1990; Carstensen 2001; Müller 1997, 1998) for the connection between Young measures and microstructures.

Let α and β be particular names for referring to each one of the solid phases that the material can exhibit. We assume that the solid phase α can be present in a wide range of deformations but not in all of them; the same is true for the solid phase β. It is easy to note that a particular range of deformations can be attained by a convenient mixing of solid phases α and β. It is well known also, that high stress conditions instead of produce higher deformations can cause a phase transition from α to β into the material. See (Bhadeshia 1987; Shackelford 1996; Valencia 1998).

This observation can be easily represented into Figure 7, where the zone to the left of point A can be related to the solid phase α and the zone to the right of B can be related to the solid phase β. That means that solid phase α is appropriate for low stress conditions with low deformations, and solid phase β can withstand higher stresses and develop higher deformations without collapsing. This is just the case in FCC and BCC solid phases in steels. From an energetic point of view, solid phase α can store low levels of deformation energy while solid phase β can store high levels of deformation energy. Thus, the mixing of solid phases α and β in the proper amounts allows the material to retain lesser levels of deformation energy. This mixing process should take place precisely within the zone limited by the points A and B on the graph of ϕ, just the zone where ϕ departs from its convex envelope ϕ_c.

Since the convex combination (28) can be described by using a probability distribution, i.e. :

$$(\epsilon, \phi_c(\epsilon)) = \int_0^\infty (t, \phi(t))\, d\mu^*(t) \text{ with } \mu^*_\epsilon = p_1\delta_{\epsilon_1} + p_2\delta_{\epsilon_2}, \tag{29}$$

we can determine the theoretical microstructure of the material from the parametrized measures μ^*_x solving (5). Thus, if $\mu^*_x = \delta_{s(x)}$ the material should develop a single solid phase corresponding to the deformation $\epsilon = s(x)$ in the potential $\phi(x, \epsilon)$ at the point x. Otherwise, $\mu^*_x = p_1(x)\delta_{s_1(x)} + p_2(x)\delta_{s_2(x)}$ and the material should mix the solid phases corresponding to the deformations $\epsilon_1 = s_1(x)$ and $\epsilon_2 = s_2(x)$ at the point x, in the proportions given by the values $p_1(x)$ for ϵ_1 and $p_2(x)$ for ϵ_2.

4.2 Examples of physical models

In order to find general qualitative properties of non-linear elastic bars, we will use the polynomial

$$\frac{\partial \phi(\epsilon)}{\partial \epsilon} = 6195.87\epsilon^3 - 4664.61\epsilon^2 + 1016.64\epsilon \tag{30}$$

as a rough representation of a typical non-linear strain-stress curve of one industrial material. This polynomial is shown as the continuous line in Figure 6. By elementary integration we obtain the fourth degree polynomial

$$\phi(\epsilon) = 1548.97\epsilon^4 - 1534.87\epsilon^3 + 508.319\epsilon^2 \tag{31}$$

which can be used as a model for the deformation energy potential of the material. See Figure 7.

4.3 Example 5

Here we solve the variational problem

$$\begin{aligned}&\min_u \int_0^1 \left\{\phi(u') + u(x)^2\right\} dx \\ &\text{s.t.} \;\; u'(x) \geq 0 \quad \text{for every } x \in [0,1] \\ &\qquad u(0) = 0, \quad u(1) = \tfrac{1}{4},\end{aligned} \tag{32}$$

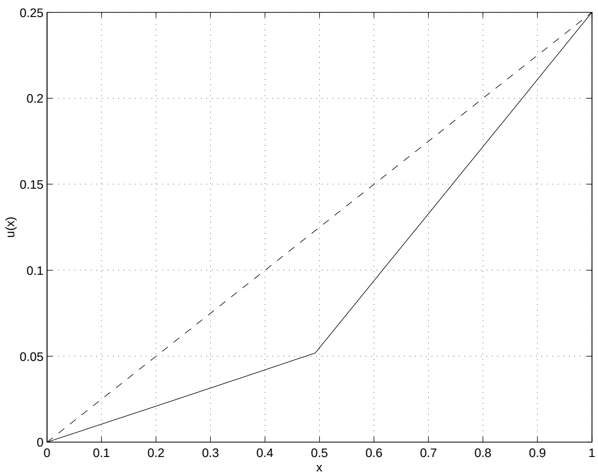

Fig. 8 Estimated minimizer for problem (32), the dashed line is $u(x) = \frac{1}{4}x$.

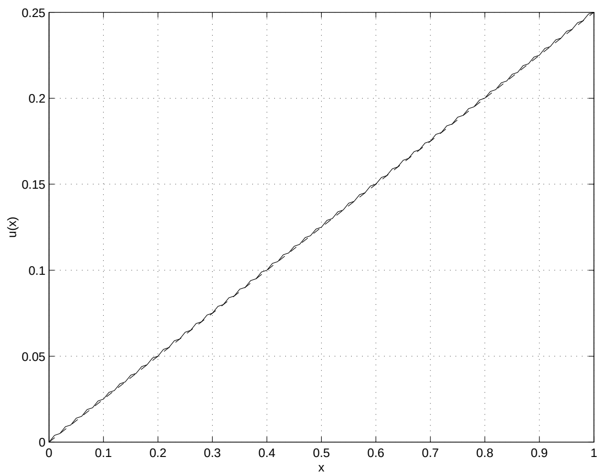

Fig. 9 Minimizing sequence for problem (35), the dashed vertical line is $u(x) = \frac{1}{4}x$.

where the non-convex, deformation energy potential ϕ is given as the polynomial in (31) and shown in Figure 7. We remark that ϕ is a fourth degree polynomial used as a rough model for the deformation energy potential of low carbon steels. Thus, we can apply the method of moments to analyse the non-convex formulation (32) which is transformed into the following convex optimal control problem:

$$\begin{array}{l} \min\limits_{\mathbf{m}} \int_0^1 \left\{ c_2 m_2(x) + c_3 m_3(x) + c_4 m_4(x) + u(x)^2 \right\} dx \\ \text{s.t. } \; u'(x) = m_1(x), \\ \qquad \begin{pmatrix} 1 & m_1(x) & m_2(x) \\ m_1(x) & m_2(x) & m_3(x) \\ m_2(x) & m_3(x) & m_4(x) \end{pmatrix} \geq 0, \\ \qquad \begin{pmatrix} m_1(x) & m_2(x) \\ m_2(x) & m_3(x) \end{pmatrix} \geq 0, \\ \qquad \text{for every } x \in [0,1] \end{array} \tag{33}$$

with $c_2 = 508.319$, $c_3 = -1534.87$ y $c_4 = 1548.97$. From the numerical solution of (33) we conclude that the optimal parametrized measures are:

$$\begin{array}{lll} \mu^*_{x_i} = \delta_{0.106} & for & i = 1, ..., 25 \\ \mu^*_{x_i} = \delta_{0.390} & for & i = 26, ..., 50 \end{array} \tag{34}$$

and herein that the problem (32) might has a minimizer as the one shown in Figure 8. In this case there is no mixing of solid phases in the body. Instead, the solid phase α is developed into the zone $\left[0, \frac{1}{2}\right]$ and the solid phase β is developed into the zone $\left(\frac{1}{2}, 1\right]$. This is the best energetic stable configuration for the variational model (32).

4.4 Example 6

By using the deformation energy potential ϕ given in (31), we can solve the variational problem:

$$\begin{array}{l} \min\limits_{u} \int_0^1 \left\{ \phi(u') + \left(u(x) - \frac{1}{4}x\right)^2 \right\} dx \\ \text{s.t.} \\ u'(x) \geq 0 \quad \text{for every } x \in [0,1] \\ u(0) = 0, \quad u(1) = \frac{1}{4} \end{array} \tag{35}$$

to obtain the Young measure solution:

$$\mu^*_{x_i} = 0.493\delta_{0.106} + 0.507\delta_{0.390} \text{ for every } i = 1, \ldots 50 \tag{36}$$

from which we conclude that problem (35) lacks of minimizers in $H_0^{1,4} + g_0$. Notwithstanding, we can determine the general form of its minimizing sequences. See Figure 9. From these results, we can see that in this model the mixing of solid phases α and β takes place in the proportions 49.3% to 50.7% all along the body. Thus, we find the best energetic configuration and therein the most stable and predictable microstructure for the body.

4.5 Conclusions

In this work we propose a practical method called the *method of moments* which is intended to determine optimal Young measures solving the generalized formulation of (1) when the deformation energy potential ϕ is a polynomial. In this way we determine either minimizers or minimizing sequences of (1). On the other hand, we can apply this method to study qualitative and quantitative features of models of energetic balances of one-dimensional, non-linear elasticity problems given in the form (1). Thus, we find the specific way in which two solid phases combine to form the microstructure of the body. This approach is enlightening when applied upon models of materials that exhibit fluence and hardening owed to internal solid phase transitions as is the case in several kinds of commercial steels.

5 Appendix: Theoretical Facts of the Method of Moments

In this appendix we give the essentials of the theory of moments when applied to non-convex variational problems with restrictions on the derivative like: (1). See (Egozcue et al 2003).

Theorem 1 *The minimum value of the optimal control problem (8) coincides with the infimum of the variational problem (1) when the potential ϕ has the form given in (2).*

Theorem 2 *Let $\mathbf{m}^*$ be a minimizer of the optimal control problem (8). Then, the entries of every vector $\mathbf{m}^*(x)$ are the algebraic moments of the optimal parametrized measure μ_x^* within an optimal Young measure solving the generalized formulation (5).*

We briefly remark here on how the unicity of the solution affects the analysis of the problem. There are situations in which the variational formulation admits several minimizers but its relaxation in moments admits only one. As instance consider

$$\begin{array}{ll} \min\limits_{u} & \int_0^1 \{(1-u'(x)^2)^2\}dx \\ \text{s.t.} & u' \geq 0 \\ & u(0)=0,\ u(1)=0.5. \end{array} \tag{37}$$

We analyze here situations in which the non-convex variational formulation lacks of minimizers but its relaxation in moments admits one. This fact is owed to the convex structure of the relaxation in moments and the coercivity of ϕ at the integrand of the functional. Certainly, we can easily find particular cases in which the relaxed formulation in moments admits several minimizers. Nonetheless, we never can expect lacking of minimizers in the relaxed formulation as it is its main purpose: to give us a convex setting where we can calculate minimizers.

5.1 Proofs of Theorems 1 and 2

The core of these proofs is the analysis of convex envelopes of polynomials f defined on the semi-axis $[0,\infty)$ as has been recently proposed in (Ben-Tal and Nemirovski 2001; Egozcue et al 2001, 2003; Meziat 2003a,b). Essentially, for an arbitrary point $t \geq 0$ we must determine points $t_1, t_2 \geq 0$ and values $p_1, p_2 \geq 0$ which make true the following expression:

$$(1, t, f_c(t)) = p_1\,(1, t_1, f(t_1)) + p_2\,(1, t_2, f(t_2)) \tag{38}$$

whose integral form is:

$$(1, t, f_c(t)) = \int_0^\infty (1, \lambda, f(\lambda))\; d\mu^*(\lambda) \tag{39}$$

where

$$\mu^* = p_1\delta_{t_1} + p_2\delta_{t_2} \tag{40}$$

and δ_t is a Dirac measure supported in t. By using convex analysis, we can define μ^* as the solution of the following optimization principle:

$$f_c(t) = \min_{\mu} \int_0^\infty f(\lambda)\, d\mu(\lambda) \tag{41}$$

where μ represents the family of all probability distributions supported in $[0,\infty)$ with mean t. See (Rockafellar 1970). If f can be described as a coercive polynomial given in the general form:

$$f(t) = \sum_{k=0}^{K} c_k t^k, \quad c_K > 0, \quad K > 1 \tag{42}$$

then we can transform the optimization problem (41) into the semidefinite program:

$$\begin{array}{ll} \min\limits_{\mathbf{m}} & \sum\limits_{k=0}^{K} c_k m_k \\ \text{s.t.} & H_1 = (m_{i+j})_{i,j=0}^{\frac{K}{2}} \geq 0, \\ & H_2 = (m_{i+j+1})_{i,j=0}^{\frac{K}{2}-1} \geq 0 \\ \text{with} & m_0 = 1, \\ \text{and} & m_1 = t \end{array} \tag{43}$$

when K is even. An analogous result holds for odd K by putting H_3 and H_4 Hankel matrices of (9) into the places of H_1 and H_2 in (43). The following lemmas tell us how to use convex optimization to solve the optimization problem (41) and how to find the values t_i and p_i in (40).

Lemma 1 *The solution $\mathbf{m}^*$ of the semidefinite program (43) is the vector formed by the first $K+1$ algebraic moments of the optimal measure μ^* given in (40), which solves the optimization problem (41) at the point t.*

See (Meziat 2003a) for a proof of this lemma. Since μ^* is supported in two points at most we can construct μ^* in (40) by using its moments 1, t, m_2^* and m_3^* which can be obtained by solving the semidefinite program (43). This task can be carried out by using some algebra. See (Akhiezer 1962; Curto and Fialkow 1991; Krein 1977).

Lemma 2 *The convex envelope of the polynomial f in (42) can be written as*

$$f_c(t) = \min_{\mathbf{m}} \sum_{k=0}^{K} c_k m_k \tag{44}$$

where the feasible set for $\mathbf{m}$ is described in (43).

See (Meziat (2003b)). As shown recently in (Dacorogna 1989; Pedregal 1997), the infimum value of the variational problem (1) coincides with the minimum of the following convex relaxation:

$$\begin{aligned} &\min_{u} \int_0^1 \{\phi_c(x,u') + \psi(x,u)\}\, dx \\ &\text{s.t.}\;\; u'(x) \geq 0 \quad \text{for every } x \in (0,1) \\ &\qquad u(0) = 0,\; u(1) = \alpha \end{aligned} \tag{45}$$

which must have a minimizer $\overline{u}$. Therefore, by applying Lemma 2 we have:

$$\begin{aligned} &\int_0^1 \{\phi_c(x,\overline{u}') + \psi(x,\overline{u})\}\, dx = \\ &\min_{\mathbf{m}} \int_0^1 \left\{ \sum_{k=0}^{K} c_k(x) m_k(x) + \psi(x,u) \right\} dx \end{aligned} \tag{46}$$

where the optimization process at the right hand is the optimal control problem (8). Due to Lemma 1 and the expression (44) in Lemma 2, if the control function $\mathbf{m}^*(x)$ satisfies the optimal control problem stated at the right hand of (46), then the components of the vector $\mathbf{m}^*(x)$ are the algebraic moments of the optimal parametrized measure μ_x^*. $\square$

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