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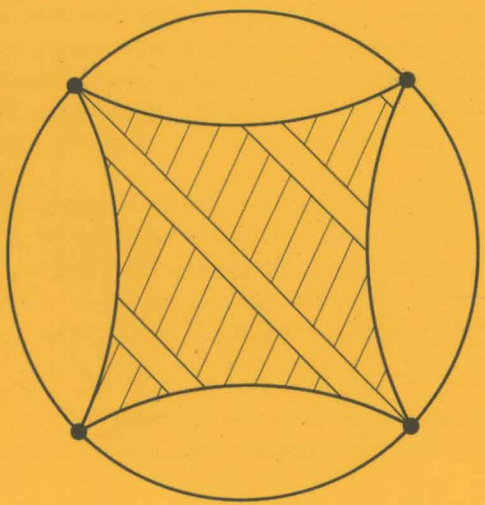
Georg Dolzmann

Variational Methods for Crystalline Microstructure – Analysis and Computation



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Variational Methods for Crystalline Microstructure - Analysis and Computation

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Preface

The mathematical modeling of microstructures in solids is a fascinating topic that combines ideas from different fields such as analysis, numerical simulation, and materials science. Beginning in the 80s, variational methods have been playing a prominent rôle in modern theories for microstructures, and surprising developments in the calculus of variations were stimulated by questions arising in this context.

This text grew out of my *Habilitationsschrift* at the University of Leizpig, and would not have been possible without the constant support and encouragement of all my friends during the past years. In particular I would like to thank S. Müller for having given me the privilege of being a member of his group during my years in Leipzig in which the bulk of the work was completed.

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College Park, August 2002 *Georg Dolzmann*

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1. Introduction

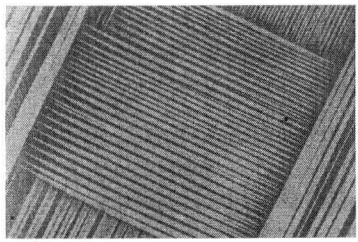
Many material systems show fascinating microstructures on different length scales in response to applied strains, stresses, or electromagnetic fields. They are at the heart of often surprising mechanical properties of the materials and a lot of research has been directed towards the understanding of the underlying mechanisms. In this text, we focus on two particular systems, shape memory materials and nematic elastomers, which display similar microstructures, see Figure 1.1, despite being completely different in nature. The reason for this remarkable fact is that the oscillations in the state variables are triggered by the same principle: breaking of symmetry associated with solid to solid phase transitions. In the first system we find an austenite-martensite transition, while the second system possesses an isotropic to nematic transition.

An extraordinarily successful model for the analysis of phase transitions and microstructures in elastic materials was proposed by Ball&James and Chipot&Kinderlehrer based on nonlinear elasticity. They shifted the focus from the purely kinematic theory studied so far to a variational theory. The fundamental assumption in their approach is that the observed microstructures correspond to elements of minimizing sequences rather than minimizers for a suitable free energy functional with an energy density that reflects the breaking of the symmetry by the phase transition. This leads to a variational problem of the type: minimize

$$\mathcal{J}(\boldsymbol{u}, T) = \int_{\Omega} W(D\boldsymbol{u}(\boldsymbol{x}), T)\mathrm{d}\boldsymbol{x},$$

where $\Omega \subset \mathbb{R}^3$ denotes the reference configuration of the elastic body, $\boldsymbol{x}$ the spatial variable, $\boldsymbol{u} : \Omega \to \mathbb{R}^3$ the deformation, T the temperature, and $W : \mathbb{M}^{3\times 3} \times \mathbb{R}^+ \to \mathbb{R}^+$ the energy density. The precise form of W depends on a large number of material parameters and is often not explicitly known. However, the strength of the theory is that no analytical formula for the energy density is needed. The behavior of deformations with small energy should be driven by the structure of the set of minima of W, the so-called energy wells, which are entirely determined by the broken symmetry.

These considerations lead naturally to the following two requirements for the energy density W. First, the fundamental axiom in continuum mechanics that the material response be invariant under changes of observers, i.e.,



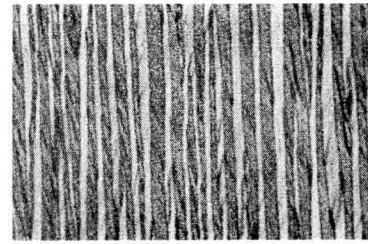


Fig. 1.1. Microstructures in a single crystal CuAlNi (courtesy of Chu&James, University of Minnesota, Minneapolis) and in a nematic elastomer (courtesy of Kundler&Finkelmann, University Freiburg).

$$W(RF,T) = W(F,T) \text{ for all } R \in \mathrm{SO}(3). \tag{1.1}$$

Secondly, the invariance reflecting the symmetry of the high temperature phase, i.e.,

$$W(R^T FR,T) = W(F,T) \text{ for all } R \in \mathcal{P}_a, \tag{1.2}$$

where $\mathcal{P}_a$ is the point group of the material in the high temperature phase. Here we restrict ourselves to invariance under the point group since the assumption that the energy be invariant under all bijections of the underlying crystalline lattice onto itself leads to a very degenerated situation with a fluid-like behavior of the material under dead-load boundary conditions. The two hypotheses (1.1) and (1.2) have far reaching consequences which we are now going to discuss briefly (see the Appendix for notation and terminology). We focus on isothermal situations, and we assume therefore that $W \geq 0$ and that the zero set K is not empty,

$$K(T) = \{X : W(X,T) = 0\} \neq \emptyset \text{ for all } T.$$

We deduce from (1.1) and (1.2) that

$$U \in K(T) \quad \Rightarrow \quad QUR \in K(T) \text{ for all } Q \in \mathrm{SO}(3),\ R \in \mathcal{P}_a. \tag{1.3}$$

This implies that $K(T)$ is typically a finite union so-called energy wells,

$$K(T) = \mathrm{SO}(3)U_1 \cup \ldots \cup \mathrm{SO}(3)U_k. \tag{1.4}$$

We refer to sets with such a structure often as multi-well sets. Here the matrices U_i describe the k different variants of the phases and k is determined from the point groups of the austenite and the martensite alone. A set of the form $\mathrm{SO}(3)U_i$ will in the sequel frequently be called energy well.

We now describe the framework for the mathematical analysis of martensitic transformations and its connection with quasiconvex hulls.

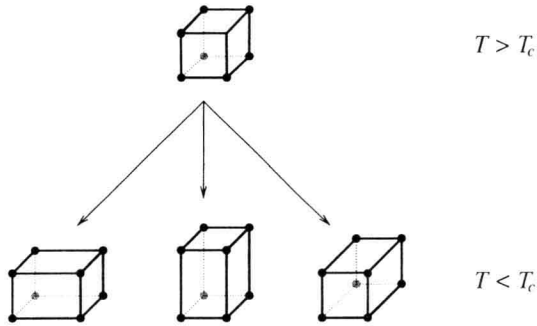


Fig. 1.2. The cubic to tetragonal phase transformation.

1.1 Martensitic Transformations and Quasiconvex Hulls

A fundamental example of an austenite-martensite transformation is the cubic to tetragonal transformation that is found in single crystals of certain Indium-Thallium alloys. The cubic symmetry of the austenitic or high temperature phase is broken upon cooling of the material below the transformation temperature. The three tetragonal variants that correspond to elongation of the cubic unit cell along one of the three cubic axes and contraction in the two perpendicular directions, are in the low temperature phase states of minimal energy, see Figure 1.2. If we use the undistorted austenitic phase as the reference configuration of the body under consideration, then the three tetragonal variants correspond to affine mappings described by the matrices

$$U_1 = \begin{pmatrix} \eta_2 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}, \quad U_2 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}, \quad U_3 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_2 \end{pmatrix}$$

with $\eta_2 > 1 > \eta_1 > 0$ (if the lattice parameter of the cubic unit cell is equal to one, then η_1 and η_2 are the lattice parameters of the tetragonal cell, i.e., are the lengths of the shorter and the longer sides of the tetragonal cell, respectively). In accordance with (1.3), the variants are related by

$$U_2 = R_2^T U_1 R_2, \quad U_3 = R_3^T U_1 R_3,$$

where R_2 and R_3 are elements in the cubic point group given by

$$R_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad R_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

A short calculation shows that no further variants can be generated by the action of the cubic point group.

The origin for the formation of microstructure lies in the fact that the different variants can coexist in one single crystal. They can be formed purely

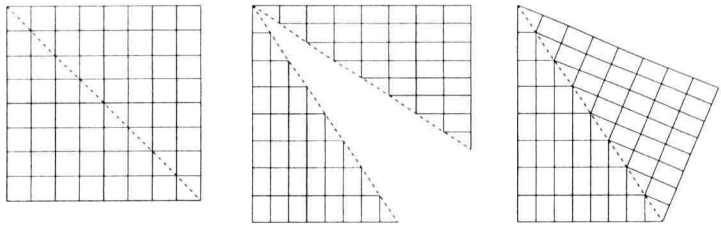


Fig. 1.3. Formation of an interface between two variants of martensite in a single crystal.

displacively, without diffusion of the atoms in the underlying lattice. This is illustrated in Figure 1.3. Consider a cut along a plane with normal $(1,1,0)$ The upper part is stretched in direction $(1,0,0)$ while the lower part is elongated in direction $(0,1,0)$. This corresponds to transforming the material into the phases described by U_1 and U_2, respectively. After a rigid rotation of the upper part, the pieces match exactly and the local neighborhood relations of the atoms have not been changed.

The austenite-martensite transition has an important consequence: the so-called shape memory effect, which leads to a number of interesting technological applications. A piece of material with a given shape for high temperatures can be easily deformed at low temperatures by rearranging the martensitic variants. Upon heating above the transformation temperature, the material returns to the uniquely determined high temperature shape, see Figure 1.4.

Mathematically, the existence of planar interfaces between two variants of martensite is equivalent to the existence of rank-one connections between the corresponding energy wells. Here we say that two wells $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$, $i \neq j$, are rank-one connected if there exists a rotation $Q \in \mathrm{SO}(3)$ such that

$$QU_i - U_j = \boldsymbol{a} \otimes \boldsymbol{n} \quad \text{(Hadamard's jump condition)}, \tag{1.5}$$

where the matrix $\boldsymbol{a} \otimes \boldsymbol{n}$ is defined by $(\boldsymbol{a} \otimes \boldsymbol{n})_{kl} = (a_k n_l)$ for $\boldsymbol{a}, \boldsymbol{n} \in \mathbb{R}^3$. If (1.5) holds, then $\boldsymbol{n}$ is the normal to the interface. More importantly, the existence of rank-one connections together with the basic assumption that the energy density W be positive outside of $K(T)$ implies that W cannot be a convex function along rank-one lines. We conclude that W cannot be quasiconvex since rank-one convexity is a necessary condition for quasiconvexity. Recall that a function $W : \mathbb{M}^{m \times n} \to \mathbb{R}$ is said to be quasiconvex if the inequality

$$\int_{[0,1]^n} W(F + D\boldsymbol{\varphi}) \mathrm{d}\boldsymbol{x} \geq \int_{[0,1]^n} W(F) \mathrm{d}\boldsymbol{x}$$

holds for all $F \in \mathbb{M}^{m \times n}$ and $\boldsymbol{\varphi} \in C_0^\infty([0,1]^n; \mathbb{R}^m)$. Quasiconvexity of W is (under suitable growth and coercivity assumptions) equivalent to weak sequential lower semicontinuity of the corresponding energy functional and