THEORY FOR THE MICROSTRUCTURE OF MARTENSITE AND APPLICATIONS

J. M. Ball (a) and R. D. James (b)

(a) Department of Mathematics, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland

(b) Department of Aerospace Engineering and Mechanics, 107 Akerman Hall, University of Minnesota, Minneapolis, MN 55455

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ABSTRACT

We present recent results on a new theory for the microstructure of martensite developed by the authors. The theory is capable of predicting the detailed patterns of microstructure that result from a martensitic transformation as well as the behavior of a martensitic crystal subject to applied loads and displacements. The crystallographic theory of martensite follows from the theory as a special case. A consequence of the theory is the extreme sensitivity of the patterns of microstructure to the precise lattice parameters, which has been explored by Bhattacharya for wedge-like microstructures appearing in shape-memory materials. We present recent predictions that relate to the deformations possible by rearranging variants and compare with experiment. Our approach is related to a theory of Khachaturyan, Roitburd and Shatalov. We explain the similarities and differences between the two approaches.

1. THEORY OF MARTENSITE BASED ON NONLINEAR THERMOELASTICITY

We briefly describe the formulation of a theory of the microstructure of martensite. The details of the derivation of this theory can be found in a recent paper (Ball and James [1991]). A central role is played by a result of Ericksen [1980] and Pitteri [1984] on Bravais lattices. A Bravais lattice is the set of points in three dimensional space of the form $\sum n^i e_i$, where n^1, n^2, n^3 are integers and $\{e_i\}$ are three linearly independent *lattice vectors*.

It is well-known that if the lattice vectors are perturbed, the point group symmetry of the Bravais lattice is lowered, as long as the perturbation is not too big. Very special perturbations may retain the same symmetry, as in the pure dilation of a cubic lattice, but a sufficiently small perturbation will never increase the symmetry. Technically, the point group of a Bravais lattice determined by the lattice vectors $\{e_i\}$ is given by

$$\{Q \in O(3): Qe_i = \mu_i^j e_j \quad \text{for some } \mu \in G\}. \tag{1}$$

Here, $O(3)$ is the set of orthogonal linear transformations and G is the group of all matrices $\{\mu_i^j\}$ with integer entries and having determinant ± 1. The Ericksen-Pitteri result says something a little

more definite than the 'lowering of symmetry' fact mentioned above; it says that a neighborhood $\mathbb{N}$ of the lattice vectors $\{e_i\}$ can be found, this neighborhood being in the 9 dimensional space of triples of vectors, such that for each $\mu \in G$ we have that $\mu\mathbb{N} = \mathbb{N}$ or $\mu\mathbb{N} \cap \mathbb{N} = \emptyset$. Furthermore, if the first alternative holds ($\mu\mathbb{N} = \mathbb{N}$) then μ necessarily corresponds to a member of the point group of the original lattice vectors $\{e_i\}$; that is, μ satisfies the equation in (1). The neighborhood $\mathbb{N}$, which we emphasize can be found for any set of lattice vectors and which depends strongly on the choice of lattice vectors, has come to be called the Pitteri neighborhood.

It turns out that the Pitteri neighborhood is an essential ingredient in writing a continuum theory for a deformable crystal that can undergo large deformations or transformation under the condition that crystal lattice deformation and continuum deformation are related through the so-called Born rule. The Born rule is the statement that deformations $y: \Omega \to \mathbb{R}^3$ of a crystal viewed as a continuum (here, Ω is the reference configuration) are related to atomic scale lattice deformations described by a deformation of the lattice vectors $e_i \to Fe_i$ by the rule

$$\nabla y(x) = F. \tag{2}$$

The Pitteri neighborhood has exactly the properties required so that, if the free energy of the lattice is assumed to depend only on atomic positions, then upon passage to the continuum theory the resulting theory has a finite symmetry group. If one decides to treat atomic scale deformations that are not included in some Pitteri neighborhood, one runs the risk of either having a continuum theory with an infinite group or one whose symmetry transformations do not form a group. Either of these possibilities is physically suspect. Partly this reflects the limitations of the Born rule, and if we knew of a good generalization of it (say, that accounted for plastic deformation), then we might see how to enlarge the Pitteri neighborhood.

Fortunately, in many materials that undergo martensitic transformations, particularly those undergoing reversible thermoelastic transformations, both the Born rule and the assumption that the deformations lie in the Pitteri neighborhood are good assumptions. As an exception, the classical BCC to FCC transformation in iron has the property that there is not a single Pitteri neighborhood that contains the lattice vectors of both lattices. At this time it is not clear to the authors how to write a continuum theory for this case.

The theory is based on the following ingredients:

1) The atomic scale free energy per unit volume is a function only of lattice vectors and temperature. This means that once the temperature and the atomic positions on the Bravais lattice are specified, then the free energy per unit volume is known. To set up the continuum theory, it is not necessary to know all the details of this function, but it is presumed frame-indifferent (i.e. the free energy per unit volume is unaffected by rigid rotations of the whole lattice).

2) The Pitteri neighborhood $\mathbb{N}$ is assumed to be based on the lattice vectors of the parent phase.

3) The lattice vectors of the martensitic phase are assumed to be contained in $\mathbb{N}$. This assumption places some restriction on the size of the transformation strain (based on a realistic choice of the Pitteri neighborhood), but this restriction is not severe in practice. The assumptions 2 and 3 necessarily imply that the point group symmetries of parent and martensitic phases are related by a group/subgroup relationship.

4) Parent and martensitic phase lattice vectors are assumed to minimize the lattice scale free energy. This assumption leads to a potential-well structure of the continuum free energy.

5) The passage from molecular to continuum theory is based on the Born rule.

The details of this derivation can be found in Ball and James [1991]; We have just sketched the argument here. The result is a continuum theory based on a free energy of the form

$$\int_{\Omega} W(\nabla y(x), \theta)\, dx \tag{3}$$

where θ is the temperature. The first argument of W is the 3x3 matrix $\nabla y(x)$, and the domain of $W(\cdot,\theta)$ is the set of all 3x3 matrices F such that Fe_i belongs to the Pitteri neighborhood $\mathbb{N}$, where e_i are the undistorted parent phase lattice vectors. If loads are applied, a potential energy of the loading device would have to be added to the expression in (3). If, on the other hand, displacement conditions are given then all deformations y(x) that compete for the minimum would have to meet these displacement conditions.

The main feature that W inherits from the lattice picture is potential wells. These are implied by the assumption 4 above. Each set of lattice vectors that minimizes the lattice free energy gives rise to a 3x3 matrix (through the Born rule) that minimizes W. Moreover, there are additional matrices that minimize W because of the fact that if g_j minimizes the lattice scale free energy than so does $\mu_i^j g_j$ for any $\mu \in G$ with $\mu\mathbb{N} = \mathbb{N}$, since both g_j and $\mu_i^j g_j$ determine the same Bravais lattice. It is a straightforward algebraic problem to calculate the resulting potential-well structure for any given sets of parent and martensitic lattice vectors.

The outline above describes how the theory is set up for transformations between Bravais lattices. Most lattices of interest are not Bravais lattices and involve atoms of different species. We have found so far that the format described above works well even in many of these cases if 1) there is a skeletal Bravais lattice which can be related to the continuum deformation through the Born rule and 2) if all changes of energy which occur are associated with a change of the skeletal lattice. A failure of the latter is most often associated with atomic scale shuffling. It is possible to work out a version of the theory for cases in which shuffling occurs, in which case W comes out depending upon additional vectors. An example of such a theory worked out for the $\alpha-\beta$ transformation in quartz is given by James [1987].

Ordering also plays a role in the behavior of shape-memory materials. An effect of ordering is to reduce the size of the group G. Apparently, this plays the role of reducing the number of potential wells outside the Pitteri neighborhood, and thereby making it more difficult for the material under stress to pass out of this neighborhood.

As an example of the final structure of the theory in a classical case, we consider the FCC to FCT transformation. It follows from the development sketched above that W exhibits a single potential well above the transformation temperature and three potential wells below the transformation temperature (these three wells continue to be present above the transformation temperature as relative minima). At the transformation temperature these wells are defined by the four matrices 1=diag(1,1,1) and

$$U1 = \begin{pmatrix} \eta 2 & & \\ & \eta 1 & \\ & & \eta 1 \end{pmatrix},$$

$$U2 = \begin{pmatrix} \eta 1 & & \\ & \eta 2 & \\ & & \eta 1 \end{pmatrix},$$

$$U3 = \begin{pmatrix} \eta 1 & & \\ & \eta 1 & \\ & & \eta 2 \end{pmatrix}.$$

It follows from frame-indifference ((1) above) that if a matrix A is on a potential well than so is every matrix of the form RA, where R is a rotation matrix. This is conveniently represented by drawing circles, although it must be appreciated that the actual "geometry of the energy wells" in 9 dimensions is more complicated. The circle attached to U_1 represents all matrices of the form RU_1, where R is a

rotation matrix. A picture of these energy wells is given in Figure 1 below; for now, ignore the dashed lines.

To find stable equilibrium configurations, we minimize the total free energy given in (3) above. We will not describe all the details of this minimization, but will just focus on some special

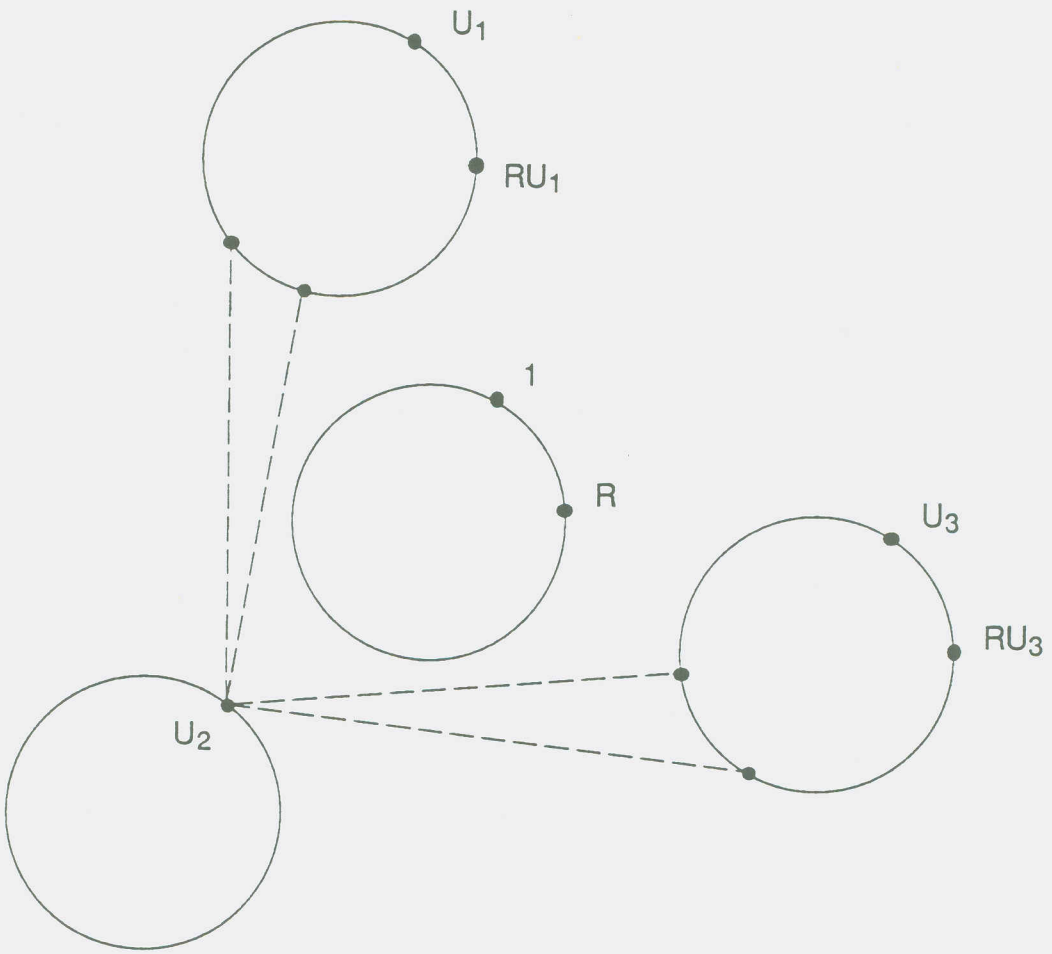


Figure 1. Cubic to tetragonal transformation. Minimizing orbits for $W(\cdot, \theta_c)$. The dashed lines summarize the rank-one connections between the variants under the conditions $\eta_2 \neq \eta_1$. The orbit attached to 1 is no longer minimizing for $\theta < \theta_c$ while the orbits attached to U_1, U_2, and U_3 are no longer minimizing for $\theta > \theta_c$, and all orbits shift slightly with temperature.

cases not involving applied loads. Obviously, in seeking a function $y(x)$ that minimizes this energy, we cannot do better than to choose $\nabla y(x)$ to take values at the minima of the potential wells at that temperature for every $x \in \Omega$. Suppose we are at or below the transformation temperature θ_c. Then, we can choose matrices A, B, C, ... on the potential well minima (i.e. on the circles in Figure 1), and put $\nabla y(x)=A$ for $x \in \Omega_1$, $\nabla y(x)=B$ for $x \in \Omega_2$, ..., where Ω_1, Ω_2,... is a subdivision of Ω. However, this is not generally possible because $\nabla y(x)$ is a gradient, i.e. the gradient of a continuous function cannot be arbitrarily assigned. In fact, two neighboring regions Ω_1 and Ω_2 can have deformation gradients A and B if and only if $B-A = a \otimes n$. Here, $a \otimes n$ is the matrix with components $a_i n_j$ and n is the normal to the interface in the reference configuration Ω. If these "rank-one connections" are satisfied between A and B, we can construct the (continuous) deformation $y(x)$, draw the image of the function $y(x)$ to get a picture of the deformation, and we can even pass back through the Born rule (2) to see how the atomic-scale lattice vectors deform.

The condition B–A = a⊗n with A and B on the potential well minima is an algebraic problem, once the locations of the wells have been assigned (a complete solution of this problem for any pair of potential wells is given by Ball and James [1987,1991]). For example, in the cubic-to-tetragonal case pictured in Figure 1, it can be shown that given any matrix on the outer circles (the 3 wells associated with the martensitic variants) there are exactly two other matrices on another martensitic well that differ from that matrix by a matrix of the form a⊗n. These are the reciprocal twins. The dashed lines in Figure 1 represent these rank-1 connections. By drawing the deformation $y(x)$, $x \in \Omega$, and passing back through the Born rule, one can verify that all of the crystallographic information about the twinning of tetragonal lattices is reproduced by this calculation of rank-one connections. For example, the normals n that emerge are the normals from the family of {110} planes. Of course, the function $y(x)$ is an energy minimizer. There are no rank-one connections between matrices on the austenite well and martensite wells. We have described here a very simple case. However, even in complicated cases all the twinning information is given automatically by straightforward algebraic calculations - Type I, Type II, or compound, the changes of shape, interfaces, etc.

There is an odd feature of the energy written down in (3). If, say, boundary values for the function $y(x)$ are given representing the action of some hard loading device, then it may happen that the minimum of the energy (3) is not attained. That is, for some boundary values, there is no function that has the property that it gives the least energy, even though the total energy is bounded from below. In such cases there are always minimizing sequences, that is, sequences of deformations whose energy gets closer and closer to the least value of the energy but which require finer and finer "microstructure" as the least value of the energy is approached. Our point of view is that such sequences model the fine microstructures observed so often in martensitic transformations. It may seem at first that there would be a great variety of such minimizing sequences, but in fact, being minimizing sequences, they are subject to strong restrictions. Our goal has been to study these minimizing sequences and to compare the results with observations.

As an example of a minimizing sequence, imagine a sequence of deformations $y^{(k)}(x)$ "trying" to assume the values A, B, and C, where A and B are on martensitic wells and B–A = a⊗n while C is on the austenite well. Since C cannot be rank-1 connected to A or B, there is no classical construction like the one described above for twins.

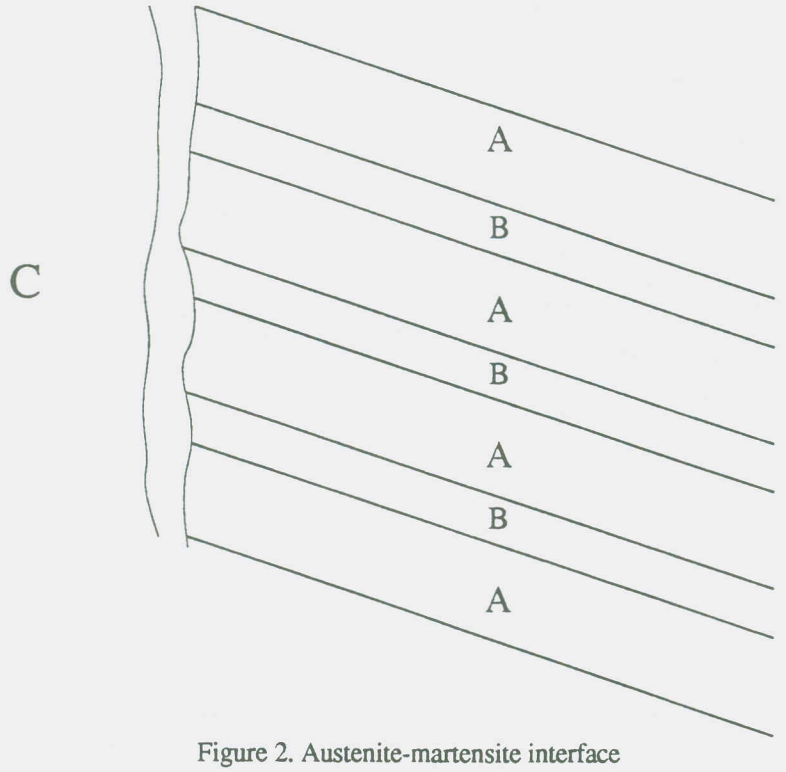


Figure 2. Austenite-martensite interface

However there is a construction closely related to the austenite/martensite interface which uses other deformation gradients besides A, B, or C, but only on sets that can be made arbitrarily small. This construction is classical and is pictured in Figure 2. Although there are no rank-one connections between austenite and martensite, it is possible to define a deformation y(x) that has the gradients pictured, as long as we are willing to interpolate y(x) through the layer between the wavy lines. This interpolated deformation will no longer have deformation gradients on the wells, so it will not be energy minimizing. However, if A, B and C satisfy special conditions and the geometry is just right, it is found that by refining the twins on the right hand side of Figure 2, the interpolated layer can be made thinner and thinner but with uniformly bounded deformation gradient. Since the gradients on the layer are uniformly bounded and since the volume of the layer goes to zero with this refinement, the construction represents a minimizing sequence for the total energy (3). The special conditions that A, B, and C must satisfy are given by

$$\begin{aligned} B-A &= a\otimes n, \\ (\lambda A + (1-\lambda)B) - C &= b\otimes m, \end{aligned} \tag{4}$$

where $0 \le \lambda \le 1$ is the volume fraction of the twins and m is a normal to the habit plane. It is easily checked by writing down the specific forms of A, B, and C (which follow from the fact that these are on the potential well minima) that the equations (4) are exactly the equations of the crystallographic theory of martensite. Again, the geometry of deformation is given by plotting the image of y(x), $x \in \Omega$, and orientation relationships and other lattice information can be discovered by passing this deformation back through the Born rule.

It is interesting to note that it is not necessary to assume the geometry of Figure 2. It can be proved (James and Kinderlehrer [1989]) that *any* minimizing sequence which involves essentially only three deformation gradients A, B and C, with A and B rank-one connected, must look like Figure 2 and C must satisfy $(4)_2$.

2. SPECIAL RELATIONS AMONG LATTICE PARAMETERS

We have looked at a number of observed microstructures and have found good agreement between the restrictions imposed by minimization and the geometry of microstructure. The most striking example has been described in the recent thesis of Bhattacharya [1990,1991]. He studies the microstructure consisting of a divided wedge with fine twins in each half, as pictured in Figure 3.

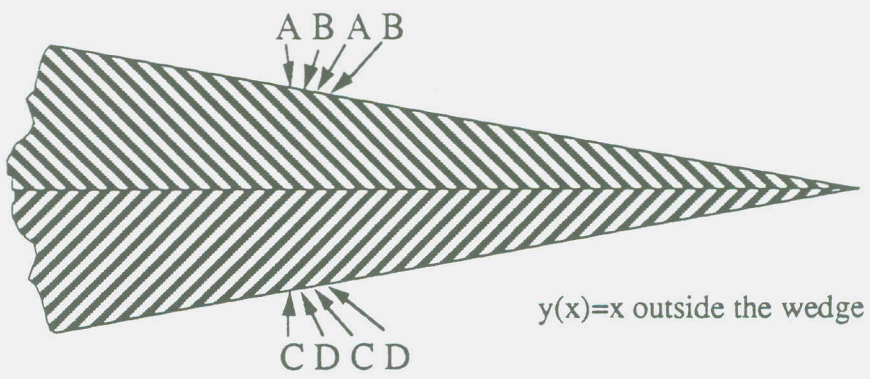


Figure 3. Wedge microstructure

This is a common microstructure in the widely studied CuAlNi alloy and other copper based alloys, but it also shows up in the shape-memory FeNiCoTi alloys. Arguably, it allows for easy transformation from a relatively small region on the boundary of a grain, which should cause less disruption to neighboring grains than transforming by a single interface transformation. The wedge microstructure can be analyzed by the methods described above. It is necessary to introduce transition layers near the boundary of the wedge and at the midrib; the energy in these layers can be

reduced to zero if and only if certain algebraic restrictions are satisfied. These restrictions always assume the form of certain rank-one connections between matrices or between convex combinations of matrices. In this case the matrices are A, B, C, D, 1, which in addition are required to lie on the potential well minima, in order that the constructed sequence be a minimizing sequence. We look at these equations in a geometric fashion. For simplicity, consider the cubic-to-tetragonal case in which the energy wells are as pictured in Figure 1. We use the following notation: a dashed line connecting two dots means that the matrices associated with those dots are rank-one connected (i.e. the difference between those matrices is a matrix of rank 1). Then a necessary and sufficient condition that the given matrices A, B, C, D, 1 can from an energy minimizing wedge is that those matrices have the rank-one connections shown in Figure 4. Even in the cubic to tetragonal case, there are a number of possibilities to analyze, because each matrix on each martensite well is rank-one connected to two others on any other martensite well. Bhattacharya [1991] has given a complete analysis.

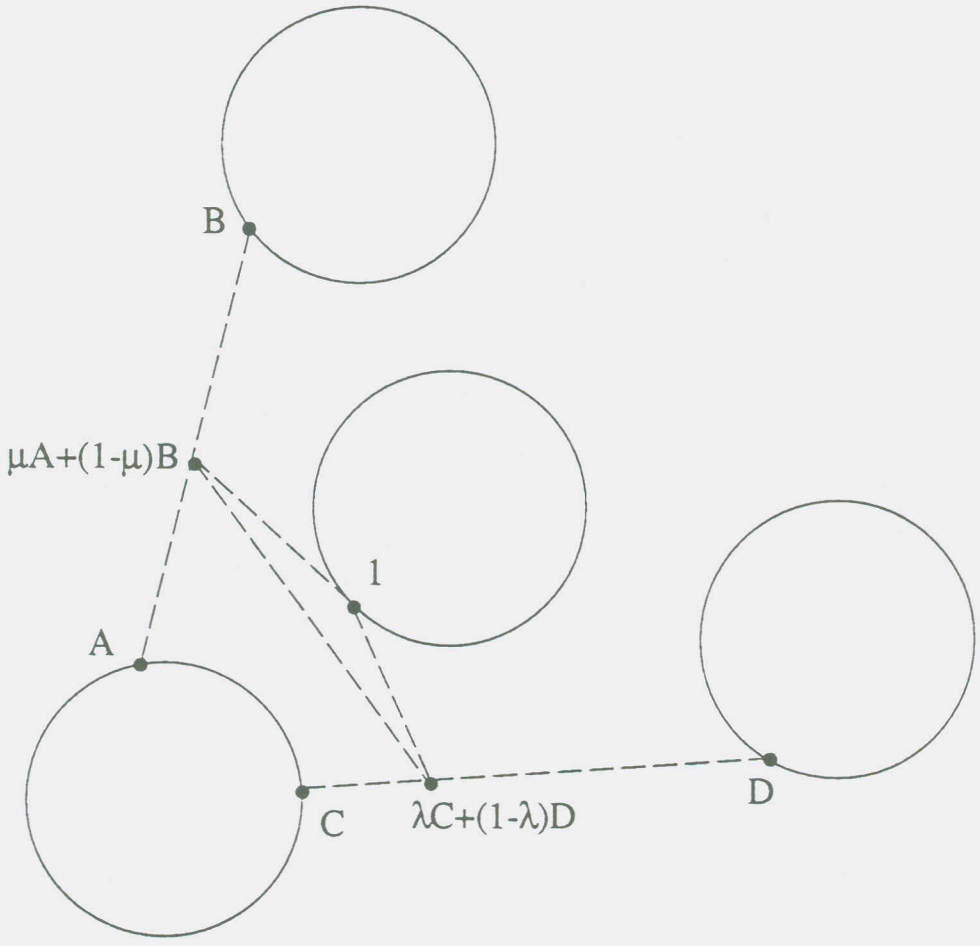


Figure 4. Rank-one connections that are sufficient for the wedge to be energy minimizing.

He also studies in detail the cubic-to-orthorhombic case which has six martensite wells. The cubic-to orthorhombic case is interesting in that, according to the present theory (and consistent with observations), some of the twins are Type II twins; if the Type I twins participate in the wedge, then the fine twins point "forward" rather than as pictured in Figure 1.

One of the surprizing results of Bhattacharya's calculations is that the set of rank-one connections given above can only be satisfied if the lattice parameters of the material satisfy certain rather restrictive conditions. In the cubic-to-tetragonal case these are restrictions on η_1 and η_2 and take the form,

$$\eta_1^2 = \{(1-\eta_2^2)^2 + 4\eta_2^2(1+\eta_2^2)\}/((1-\eta_2^2)^2 + 8\eta_2^4) \qquad (5)$$

In the cubic to orthorhombic case the relations are more complicated to write down, since there are three lattice parameters, but they are given in the form of graphs by Bhattacharya. In addition, the precise geometry of the wedge emerges from the calculation. The comparison of both the geometry and the special relations between lattice parameters with data on alloys that show the wedge is excellent.

This leads us to speculate that a factor that may be important in "good" shape-memory behavior are such special relations. It is surely true that the existence of the additional rank-one connection pictured in Figure 4 makes possible additional microstructures that would not be possible without it, and these may well be important in both easy transformation and accomodation.

Another special microstructure that is sometimes observed is the X-interface (for example, in InTl, see Basinski and Christian [1954]). The X-interface consists of four half-planes meeting at a common line, forming four wedge-shaped regions. One of the regions contains pure austenite, and the opposite one pure martensite, while the other two consist of finely-twinned martensite. Interestingly, it has been shown by Ruddock [1992] that for a cubic-to-tetragonal transformation this microstructure cannot be formed using deformation gradients at the potential well minima. This suggests that the X-interface will only be observed in specimens under stress, which seems to be consistent with observations. The KRS theory described below, on the other hand, would predict that the X-interface can be energy minimizing at zero stress if a special relation between the lattice parameters holds.

3. RELATION OF THE THEORY TO STRAIN GRADIENT THEORY

Because there is no energy in the theory accounting for the formation of interfaces, the theory treats as infinitely fine microstructures that in reality are fine but not infinitely fine. There are several advantages of this approach. First, it is relatively easy to actually compute complex microstructures, and Collins and Luskin [1989] have made considerable progress in this area. Second, the theory gives a good understanding of the conditions under which fine structure *must* occur. Third, while most of the discussions above concern microstructures at zero energy, the theory is well adapted to study the effect of loads.

However, while the theory gives the volume fractions of the finely twinned variants, it does not predict the actual thickness of the twinned layers. This is most often thought to be associated with surface energy and is often modeled by a strain gradient theory. Here, we briefly describe the position of the present theory within a strain gradient theory. A common strain gradient theory would have a free energy of the form,

$$\int_{\Omega} \left[W(\nabla y(x),\theta) + cq(\nabla\nabla y(x)) \right] dx \tag{6}$$

where q is a positive definite quadratic function of $\nabla\nabla y(x)$ that is invariant under the appropriate symmetry and frame-indifference transformations. Here, c is a typical surface energy coefficient. Barsch, Horovitz and Krumhansl[1987, 1991] have deduced forms of q that are appropriate. To understand the role of q it is useful to first write the energy (6) for a domain $\lambda\Omega$, where we think of Ω as a fixed "standard domain". Then change variables so that the energy of $\lambda\Omega$ is expressed as an integral over Ω. Writing $z(x)=\lambda^{-1}y(\lambda x)$, we have

$$\text{energy of } \lambda\Omega \;=\; \lambda^3 \int_{\Omega} \left[W(\nabla z(x),\theta) + \lambda^{-2} cq(\nabla\nabla z(x)) \right] dx. \tag{7}$$

Hence, the energy of $\lambda\Omega$ is the same as the energy of Ω, except that the surface energy coefficient c now is $\lambda^{-2}c$. We can ignore the factor λ^3 in front of the integral because for energy minimization we are only interested in energy differences.

If λ is very small, that is the domain $\lambda\Omega$ is very small, the energy of $\lambda\Omega$ is equivalent to the energy of the standard domain Ω with a very large surface energy coefficient. The positive definite term which multiplies $\lambda^{-2}c$ must then be small for any observed configuration $z(x)$, because otherwise the configuration would involve a large energy. Hence with small λ we are led to consider a constrained theory in which we impose the constraint $\nabla\nabla z(x)=0$, i.e. the deformation gradient $F(x)=\nabla z(x)$ is independent of x. Then we would go back to the integral (7) and minimize the left-over energy (the bulk energy) under this constraint. This of course leads to an easy problem involving homogeneous configurations, whose solutions could be easily understood. The idea of this calculation is a recurring theme in continuum mechanics and goes back at least as far as Stoner and Wohlfarth's theory of the ferromagnetism of small particles.

Of greater interest here is the alternative limit λ very large. In this case we are led by a similar argument to consider (7) with λ large. In this case the second term in (7) is very small and we are led to minimize first the bulk energy term in (7), which is the present theory. We then find there are several minimizers (or minimizing sequences); following the thinking presented above, we would then go back to the second term in (7) and find which of these gives the smallest surface energy. Thus, the present theory applies to large specimens.

The question remains: how large is "large"? Some indication is provided by recent experiments of Miyazaki [1991] on thin films of TiNi. He finds that films that are on the order of 10 μm thick still exhibit stress-strain-temperature curves that are similar to mm or cm size specimens, although there are some small but noticeable differences. We are now looking at these kinds of scaling arguments for thin rods and thin plates (in which the appropriate scaling is not a dilatation as discussed above) to see what kinds of theories emerge.

4. RELATION TO THE THEORIES OF KHACHATURYAN, SHATALOV, AND ROITBURD

Over the last 25 years a different theory designed to predict the morphology of crystal microstructure via energy minimization has been developed by Khachaturyan [1967, 1983], Roitburd [1967, 1978] and Khachaturyan and Shatalov [1969]. This theory has several ingredients in common with ours; for example, interface orientations are calculated by seeking rank-one connections between energy wells, a link is made with the crystallographic theory of martensite (Khachaturyan [1983, p. 380]), and multiple layering is identified as a mechanism for energy reduction (*cf.* Khachaturyan and Shatalov [1969] and the 'polydomain plates' of Roitburd [1978]). In a recent paper Kohn [1991] has shown that the Khachaturyan-Roitburd-Shatalov (KRS) theory can, roughly speaking, be thought of as a 'linearization' of the present theory in which the displacement $u(x)=y(x)-x$ is assumed small, and the free energy function $W(\nabla y, \theta)$ is replaced by the function

$$W_{lin}(e) = \min_{1\le i\le N} \left\{ w_i + \frac{1}{2}\langle \alpha_i(e-E_i), e-E_i\rangle \right\} \qquad (8)$$

of the linearized strain $e=e(u)=\frac{1}{2}(Du+(Du)^T)$. In (8) α_i represents the tensor of linear elastic moduli of the i^{th} phase, $E_i=E_i^T$ is the stress-free strain of the i^{th} phase, and w_i its energy. Thus the energy wells (e.g. Figure 1) of the nonlinear theory are replaced by the set

$$M_{lin} = \{A\in M^{3\times 3}: \tfrac{1}{2}(A + A^T) = 1 + E_i \quad \text{for some } i=1, \ldots, N\} .$$

Note that the energy W_{lin} in (8) is not quadratic, so that the KRS theory is still *nonlinear*, in contrast to usual linearized theories of elasticity. In order to give it a status with respect to the present theory (which does not assume small displacements and in particular does not linearize rotations), it appears

to be necessary to assume that for each x the distance of the deformation gradient $\nabla y(x)$ from the set of potential well minima scales in a particular way with respect to $\max_{1\le i\le N} |U_i - 1|$, which is itself small.

A detailed comparison between the KRS and the present approach is given by Ball and James[1991] so we shall just make a few remarks here. If the transformation strain is small, the two approaches predict nearly the same interface normals, either for austenite-martensite interfaces or for the twin interfaces, except in some unusual situations. Some twin interfaces which are predicted to be slightly irrational by the KRS theory are exactly rational by the present theory, but the differences are slight for realistic values of the lattice parameters. The KRS theory predicts that the wedge microstructure is not possible, i.e. the wedge angle must be zero by KRS theory. This is expected based on the fact that materials that form the wedge have large transformation strain. There are some boundary conditions that can be accomodated by several microstructures in the KRS theory but which have a unique energy minimizing microstructure according to the present theory. Thus the nonlinear theory breaks a kind of degeneracy present in the linear theory.

Finally, for deformations involving large rotations (such as in rods) the two theories can give dramatically different results. To see this, consider two variants specified by two matrices $S^{\pm}=1\pm\delta e_2\otimes e_1$ describing shears (it can be shown that by a linear change of variables, any pair of variants can be put into this form). Using the notation for the wells given above, we have the two variants shown in Figure 5.

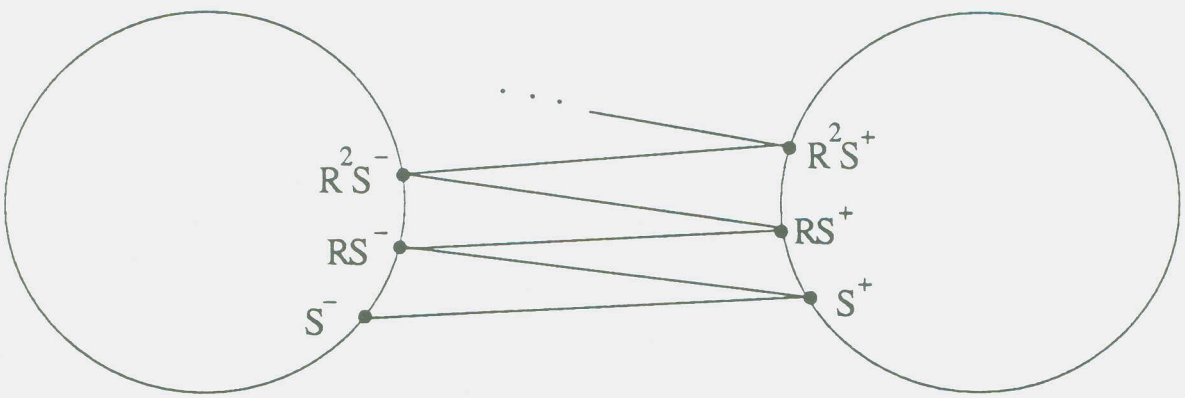
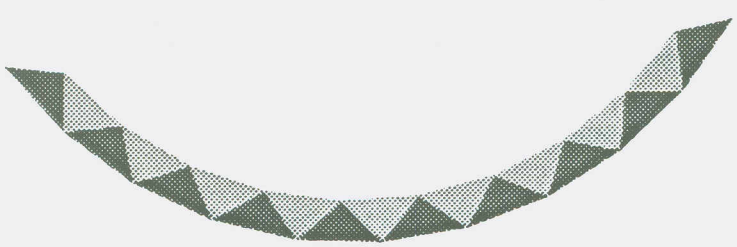


Figure 5. Two variants showing rank-one connections

A sequence of rank-one connections is shown in Figure 5; this is easily built up using the result mentioned above that each matrix on one variant well is rank-one connected to exactly two matrices on another variant well. This sequence of rank one connections implies that a deformation exists with the indicated matrices, and in fact this deformation is a minimizer of energy for a free crystal. Physically, this deformation represents an alternating set of twins and reciprocal twins. In the KRS theory (8) we can also find an energy minimizing deformation with alternating twins and reciprocal twins. Suppose we do this using a KRS theory based on the same choice of transformation strain $S^{\pm}=1\pm\delta e_2\otimes e_1$. With $\delta = 0.1$ (a realistic choice for shape-memory materials) we get the two deformations shown in Figure 6.



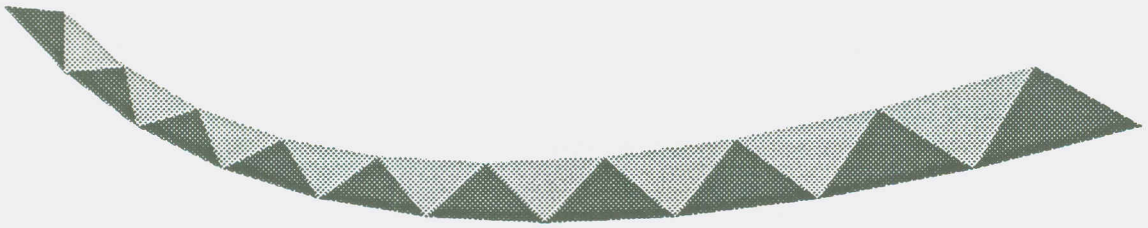


Figure 6. Deformations of a rod using KRS and the present theory. The present theory gives the circular shape.

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