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BIFURCATIONS IN BRAVAIS LATTICES

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WORKSHOP ON CALCULUS OF VARIATIONS AND
NONLINEAR MATERIAL BEHAVIOR
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Outline

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J. L. Ericksen

Commonly, Martensitic transformations associated with shape memory effects are of first order. It seems typical that, as one cools one in the austenitic phase which is stable at higher temperatures, some elastic modulus becomes unusually small, seeming to extrapolate to zero, at a temperature slightly below the transition temperature. Although there is little evidence to support it, there is some opinion that a similar effect should occur, as one warms the Martensite which is stable at lower temperatures. This raises a question which has intrigued me. Experience with bifurcation theory suggests that, if we accept that those moduli do vanish, one there has a bifurcation, involving equilibrium branches which seem to be too unstable to be observable. So, what can we infer, theoretically, about the qualitative features of such bifurcations, from what can be observed?

What is proving to be useful in describing at least some of the near-transition behavior of such materials is the nonlinear thermoelasticity theory of Bravais lattices. This involves a Helmholtz free energy function, hereafter called the potential, which is invariant under an infinite discrete group. However, the restriction of this to a suitable neighborhood of any configuration is invariant only under a finite group, the point group associated with this configuration. For our purposes, equilibria can be considered as homogeneous, unstressed configurations. Then, for local bifurcation theory, we can consider the potential to be invariant under the point group for the configuration occurring at bifurcation. Logically, this could be any of the seven point groups which can be realized in Bravais lattices, and my goal is to construct a fairly general theory of these. At least for a first look, I'll assume that the potentials are smooth. Also, I will use an old idea, still in common use among physicists, to reject as unlikely some of the numerous mathematical possibilities.

I'll sketch my plan of attack, which is pretty much that commonly used in bifurcation theory. The potential will be considered as a smooth function of the usual Cauchy-Green tensor C and θ. The aim is to solve the equilibrium equations (zero-stress condition) for C as a function of θ. So, one considers a solution at a particular value of θ, and tries to apply the implicit function theorem. What is important for this is a fourth order tensor obtained by differentiating the potential twice with respect to C or, what is equivalent, the tensor A of linear elastic moduli, considered as a (symmetric) linear transformation on the space of second-order symmetric tensors. If kerA=0, the implicit function theorem applies, giving us the local existence and uniqueness of smooth solutions, nice equilibrium branches. On these, it is not hard to show that the point group of configurations remains fixed. For bifurcation theory, one is interested in equilibria which are limit points of such branches, at which A has a nontrivial kernel. By a simple continuity argument, the point group at a limit point of a branch must either be or contain as a subgroup that on the branch.

On a branch, various functions of interest related to the potential, such as A, reduce to functions of θ. As a consequence of invariance, these will automatically satisfy some equations. The aforementioned criterion is that one additional equation might well be satisfied at a particular value of θ, but it is very unlikely that two or more independent equations are satisfied simultaneously.

In a conventional way, we can define the eigenvectors and eigenspaces of A. As a consequence of invariance, A will be invariant under the point group associated with the configuration at which it is evaluated, which can force two or more eigenvalues to coincide. Necessarily, the eigenspaces are invariant under this group. If the number of distinct eigenvalues is as large as it can be, these spaces are also irreducible. That is, they contain no proper subspaces which are also invariant under the group. To have a non-trivial kernel, at least one eigenvalue of A must vanish, giving one equation to be satisfied. By the aforementioned criterion, it is then unlikely that any two eigenvalues will also be equal, unless this is forced by invariance. So, the

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eigenspaces, in particular the kernel, are irreducible spaces and, of course, such eigenspaces are orthogonal to each other. By using these properties, one can get useful characterizations of the eigenvalues and eigenspaces, for the various point groups. After some calculation, one finds that the possible dimensions of eigenspaces are one, two or three. It is pretty clear that the qualitative character of bifurcations will depend somewhat on the point group involved and, then, on which of the different eigenvalues vanishes, at least. I'll sketch my my strategy for helping to reduce the numerous possibilities to a manageable list of mathematical problems.

To proceed, it is convenient to introduce an orthonormal basis of eigenvectors of A, evaluated at a putative bifurcation point, to serve as a basis for symmetric second order tensors, in particular, values of C. Using the implicit function theorem, one can solve the equilibrium equations for some components of C in terms of the others and θ. By substituting this into the potential, one gets the reduced potential, a function of a smaller number of deformation variables, equal in number to the dimension of the kernel. Essentially, these are what are called "order parameters" by physicists. Using the implied uniqueness, one can determine what invariance the reduced potential inherits. Also, from the way it is defined, the first and second derivatives of the reduced potential with respect to the order parameters vanish, when evaluated at the bifurcation point. By the procedure described, and with the order parameters interpreted as rectangular Cartesian coordinates, the latter invariance groups turn out to be finite subgroups of the orthogonal group in one, two or three dimensions, making it easier to relate these bifurcations with some occurring in other kinds of applications.

In one dimension, either the group consists of the identity or it also includes reversing the sign of the variable. In the two-dimensional case, one gets groups generated by a rotation with angle $\pi/3$, $\pi/2$ or $2\pi/3$ and an improper transformation. With a suitable choice of the basis of eigenvectors, the latter is represented by the matrix

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

There is just one three-dimensional case, associated with the cubic group, described below. For this, my calculations give a group of order 24, generated by two improper transformations: use the negatives of two rotations with angle $\pi/2$, about two different crystallographic axes. So, the reduced potential is a function which is invariant under one of these six groups. Analyzing the likely bifurcation patterns for the six is a manageable task. This, along with a chart linking these to the original physical possibilities, provides pictures of what I would regard as typical bifurcation patterns in Bravais lattices.

Here, I won't try to elaborate the bifurcation patterns produced by analyses of all the possibilities. I have not made a thorough search of the literature on bifurcation theory, so can't exclude the possibility that all of these analyses are presented somewhere in it. Certainly, some are.

A very commonly observed possibility has as Austenite a cubic crystal. Since the cubic group is maximal, a limit point also has this symmetry. With the usual choice of crystallographic vectors as an (orthonormal) basis, and with the bifurcation point taken as a reference, the eigenspaces mentioned above are as follows.

a) one-dimensional; tensors proportional to 1.
b) two-dmensional; traceless tensors of diagonal form
c) three-dimensional; tensors with zero diagonal components.

Observations indicate that it is the eigenvalue associated with the two-dimensional space which vanishes. With the implicit functional theorem, it is easy to show that nearly equilibria will have zero off-diagonal components, so it suffices to consider only those of diagonal form. For these, one orthonormal basis of eigenvectors is given by

$$\sqrt{2}\ E_1 = \mathrm{diag}\,(1, -1, 0)$$
$$\sqrt{6}\ E_2 = \mathrm{diag}\,(1, 1, -2)$$
$$\sqrt{3}\ E_3 = \mathrm{diag}\,(1, 1, 1)\,.$$

Assuming C is diagonal, we can write

$$C = \sum_{i=1}^{3} x_i E_i ,$$

and, with the implicit function theorem, we can solve the equilibrium equations for x_3, in terms of x_1, x_2 and θ, using this to get a reduced potential function of the form $F(x_1, x_2, \theta)$. At bifurcation $\theta=\theta_B$, $x_1=x_2=0$, we will have

$$\frac{\partial F}{\partial x_i} = \frac{\partial^2 F}{\partial x_i \partial x_j} = 0 , \quad i, j = 1 \text{ or } 2.$$

To calculate the group leaving F invariant, we proceed as follows. Let Q be any of the 3×3 matrices describing the cubic group: it transforms C into QCQ^T, taking diagonal tensors to diagonal tensors. Calculate the quantities λ_i^j such that

$$QE_iQ^T = \sum_{j=1}^{3} \lambda_i^j E_j .$$

Since E_3 and the pair (E_1, E_2) lie in different invariant subspaces, one gets relations like $\lambda_1^3=\lambda_2^3=0$, and, with E_i orthonormal, one finds that the matrices

$$\begin{Vmatrix} \lambda_1^1 & \lambda_2^1 \\ \lambda_1^2 & \lambda_2^2 \end{Vmatrix}$$

are orthogonal. Then, with

$$QCQ^T = Q\left(\sum_{i=1}^{3} x_i E_i\right) Q^T = \sum_{i,j=1}^{3} x_i \lambda_i^j E_j$$
$$= \sum_{j=1}^{3} \bar{x}_j E_j ,$$

from which one can read off the transforms of x_1 and x_2, which is also the invariance group for F. This works out to be the group generated by a 120° rotation and the improper transformation

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

With F invariant under this group, it is easy to show that

$$x_1 = x_2 = 0 \Rightarrow \frac{\partial F}{\partial x_1} = \frac{\partial F}{\partial x_2} = 0\,,$$

which describes a cubic equilibrium branch, passing smoothly through the bifurcation point. Clearly, F is an even function of x_1, so

$$x_1 = 0 \Rightarrow \frac{\partial F}{\partial x_1} = 0\,.$$

I won't belabor the analysis, but, by a fairly elementary exercise in bifurcation theory, one can deduce that the likely possibility is that the other equilibrium equation has a solution of the form $x_1=0$, $x_2=f(\theta)\neq 0$, $f(\theta)$ being a smooth function, vanishing at the bifurcation temperature. Applying the invariance group to this gives three symmetry-related branches of this kind: physically, these are crystal configurations with tetragonal symmetry. I did consider the possibility of having additional branches, finding that this is unlikely. In terms of the aforementioned observations, one expects all eigenvalues to be positive on the cubic branch, for θ greater than the value θ_B at bifurcation. According to my analyses, one is negative on each of the other branches, indicating that these are quite unstable. So, this gives some impression of what kinds of results can be obtained to characterize the more likely kinds of bifurcation patterns in Bravais lattices.

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13. ABSTRACT *(Maximum 200 words)*

In unloaded crystals, it is rather common for equilibrium configurations, to undergo some change in crystal symmetry as the ambient termperature changes, in what are commonly called Martensitic transformations. Sometimes, near transition, one observes that some elastic modulus is relatively very small and there is some opinion that this is somehow related to so-called "shape memory effects" exhibited by certain crystals, for example. In this, there is a suggestion that, theoretically, the softening is associated with near approach to a bifurcation, involving equilibria too unstable to be observed. The problem considered as to ascertain what can be said about the character of such unstable paths, given certain properties of the stabler paths. To be covered is some relevant local theory, which provides a qualitative description of the several kinds of patterns which can occur, generically.

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