Some Surface Defects in Unstressed Thermoelastic Solids

J. L. ERICKSEN

Dedicated to Walter Noll, on the Occasion of His Sixtieth Birthday

I. Introduction

In the literature on crystals, "twinning" is a word used to describe a variety of phenomena involving different but symmetry-related configurations which coexist in crystals, meeting to form surfaces of discontinuity. As is discussed by PITTERI [1], there have been various attempts to formulate a more precise general definition of the word, as it applies to crystals. His discussion makes clear that some types of twinning are outside the scope of thermoelasticity theory. His definition excludes some phenomena which some experts on crystals call twins, like the "rotational twins" described by BARRETT & MASSALSKI [2, p. 406], things which seem to me more reminiscent of the multiple births we commonly describe by other words, like triplets or sextuplets. Whatever one calls them, they are of physical interest, as are other somewhat similar phenomena. My purpose is to present elements of thermoelasticity theory for things of this general kind.

II. Thermoelastic Bodies

To abstract features which seem significant, we consider a homogeneous thermoelastic body, referred to a homogeneous reference configuration. For present purposes, it is characterized by one smooth constitutive equation, of the form

\[ \phi = \phi(C, \theta), \] (2.1)

with \( \phi \) identified as the Helmholtz free energy per unit mass, \( \theta \) as absolute temperature and

\[ C = F^T F = C^T. \] (2.2)

Here, \( F \) is the usual deformation gradient, with

\[ \det F > 0, \] (2.3)
implying that \( C \) is positive definite. To discuss symmetry-related configurations we want there to be some non-trivial material symmetry, so we require that

\[
\phi(H^TCH, \theta) = \phi(C, \theta), \quad H \in G,
\]

(2.4)

\( G \) being some non-trivial subgroup of the unimodular group. For crystals, molecular theory suggests for \( G \) a group which can be represented by the unimodular matrices of integers, as is discussed by ERICKSEN [3], and the experience is that this is an apt choice for analyses of twinning, etc. The \( H \) then representing \( G \) need not be these matrices of integers, but are similar to them. Select subgroups can suffice for particular problems. For general discussion, we need not fix any particular choice of \( G \).

For any particular choice of \( \theta = \theta_1 \), \( C = C_1 \) is a natural state provided the inequality

\[
\phi(C, \theta_1) \geq \phi(C_1, \theta_1)
\]

(2.5)

holds in the strict sense, at least when \( C - C_1 \) is small enough. In more physical terms, these are stable or metastable unstressed equilibrium configurations, equilibrium of the simplest kind. With (2.4), for any \( H \in G \), \( H^T C_1 H \) is also a natural state. Many studies of thermoelasticity theory presume that

\[
H^T C_1 H = C_1 \quad \forall \ H \in G.
\]

(2.6)

The group suggested above for crystals leaves invariant no symmetric, positive tensor so, with this choice of \( G \), (2.6) cannot be satisfied. Even if we ignore this, it is necessary to deny (2.5), to accommodate common examples of twinning. So we want \( \phi \) to be such that, for some \( H \in G \), and some natural state \( C_1 \),

\[
C_2 = H^T C_1 H = C_1, \quad \det H = 1,
\]

(2.7)

giving us at least two different, symmetry-related natural states. Alternatively, if \( F_1 \) and \( F_2 \) are any deformation gradients corresponding to \( C_1 \) and \( C_2 \), as indicated by (2.2) and (2.3), there exists a rotation \( R \),

\[
R^{-1} = R^T, \quad \det R = 1,
\]

(2.8)

such that

\[
F_2 = RF_1 H.
\]

(2.9)

One more condition is inherent in notions of phenomena like twinning, that it should be possible for such natural states to coexist, coherently, in the same body. That is, it should be feasible to regard \( F_1 \) and \( F_2 \) as values of \( F \) in adjacent regions, with \( F \) the gradient of a continuous deformation. This introduces the requirement that the classical kinematic conditions of compatibility be satisfied where the regions meet, viz.

\[
F_2 = (1 + a \otimes n) F_1.
\]

(2.10)

Here, \( n \) is the unit normal to the surface of discontinuity, in the current configuration, and \( a \) is the so-called amplitude vector. In this most elementary formulation, \( F_1, F_2, R \) etc. are constants; we are interested in the possibilities for patching together homogeneous deformations, with occasional planes of discontinuity,