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# Eshelby tensor and phase equilibrium

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## Abstract

It is shown that the Eshelby tensor fits seamlessly into the thermodynamic theory of phase transition and of equilibrium between coherent phases. In equilibrium the normal component of the Eshelby tensor is continuous at the phase boundary. A simple illustrative example of a linearly elastic incompressible solid in equilibrium with its - equally incompressible - melt is considered.

## 1 Introduction

Recently phase equilibria between solids have become an urgent subject of research, because high temperatures and strong tensile loads create phase transitions in structural elements of machines. These may be unwelcome in some cases, in others they may be desirable; in both cases we need to be able to deal with them and to calculate the shape and motion of the phase boundaries.

These phenomena are governed by the Eshelby tensor, the natural generalisation of the free enthalpy - or Gibbs free energy - in the thermodynamics of fluids: while in a fluid-fluid phase transition equilibrium requires the continuity of the free enthalpy itself. It is the normal component of the Eshelby tensor that is continuous at a coherent



phase boundary between solids in equilibrium. After early arguments by Gibbs [1] on the subject and after the pioneering work of Eshelby [2], more recent references to the Eshelby tensor and its role in thermodynamics of phase transitions were made by Heidug and Lehner [?], Truskinovsky [4], Abeyaratne and Knowles [5], Grinfeld [6], Liu [7], Schmidt [8] and others.

In the past few years the subject has been shrouded in mystery, e.g. by Maugin [9]. It has been suggested that the proper environment of the Eshelby tensor is a so-called "configurational space" which in some way is dual to the "physical space". This is not so! And the present paper was written in order to reaffirm the natural role of the Eshelby tensor in ordinary thermodynamics of phase boundaries. We stick to the simplest case here, a plane phase boundary, so that curvature and surface tension play no role. However, such effects are included in the master formula of the present paper, the generic equation of balance (1).

## 2 Equations of balance

### 2.1 Generic

We consider a material volume  $v$  cut into parts  $v_{\pm}$  by a singular surface as shown in Figure 1. The singular surface may represent a wall or a phase boundary and in general it will have thermo-mechanical properties of its own. Following [10] in notation we write a fairly general equation of balance for a generic quantity  $\Psi$  in the form

$$\int_{v^{++}v^{-}} \frac{\partial \psi_v}{\partial t} dv + \int_{f^{++}f^{-}} \left( \psi_v v_i + \Phi_i \right) e_i ds - \int_{v^{++}v^{-}} p_v dv + \int_s \left( \dot{\psi}_s + \psi_s \left( v_s^{\Delta};_{\Delta} - 2K_M v_{\perp s} \right) + v_s^{\Delta};_{\Delta} - [\psi_v] v_{\perp s} + p_s \right) ds = 0. \quad (1)$$



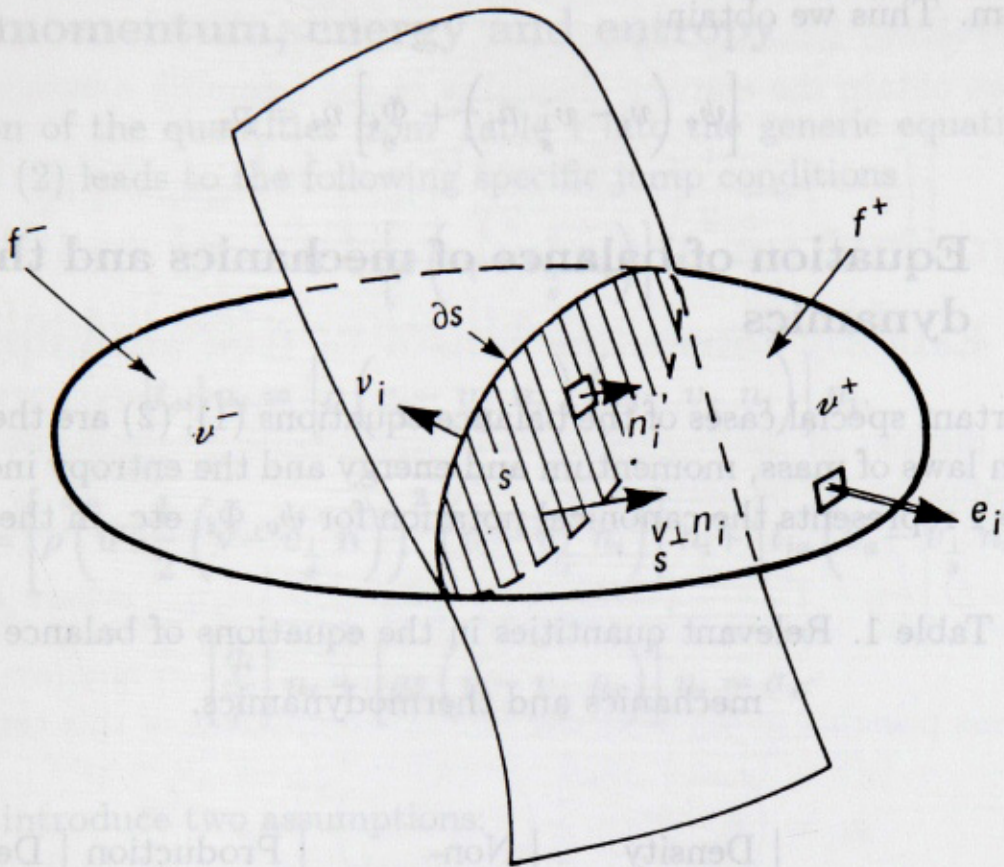


Fig. 1. Material volume cut by a singular surface.

The notation in (1) is more or less self-explanatory but for those, who are not familiar with the subject, the individual entries will be explained in the Appendix. Here we shall be interested in plane phase boundaries; these are singular surfaces of a particular type in which all terms of the second line in (1) vanish except possibly the last two.  $[\psi_v]$  is the difference of the density of  $\Psi$  on the two sides of the singular surface,  $v_{\perp s}$  is the normal speed of the surface and  $p_s$  is the surface production density.

## 2.2 Jump condition

Equation (1) may be applied to a pill box-shaped volume element with top and bottom on the two sides of the singular surface. We let the



height of the pill box tend to zero along with the areas of top and bottom. Thus we obtain

$$\left[ \psi_v \left( v_i - v_{\perp} \frac{n_i}{s} \right) + \Phi_i \right] n_i = p_s. \quad (2)$$

### 2.3 Equation of balance of mechanics and thermodynamics

Important special cases of the balance equations (1), (2) are the conservation laws of mass, momentum and energy and the entropy inequality. Table 1 represents the canonical notation for  $\psi_v$ ,  $\Phi_i$ , etc. in these cases.

Table 1. Relevant quantities in the equations of balance of mechanics and thermodynamics.

	Density of $\Psi$	Non- Convective Flux $\Phi_i$	Production per Volume $p_v$	Densities per Area $p_s$
Mass	$\rho$	0	0	0
Momentum	$\rho v_a$	$-t_{ai}$	0	0
Energy	$\rho \left( u + \frac{1}{2} v^2 \right)$	$-t_{ia} v_a + q_i$	0	0
Entropy	$\rho s$	$q_i/T$	$\sigma_v$	$\sigma_s$

Among these four quantities all but the entropy are conserved by the laws of thermodynamics so that the productions vanish. And the second law of thermodynamics requires that the entropy productions be non-negative, - positive in non-equilibrium. The momentum flux is equal to the (symmetric) stress tensor  $\mathbf{t}$  to within sign and the entropy flux is assumed to be given by heat flux  $\mathbf{q}$  divided by the absolute temperature  $T$ . The relative complexity of the energetic entries results from the fact that it is convenient to split the energy into internal and kinetic parts according to their different properties under Galilei transformations.



## 2.4 The jump conditions for the fluxes of mass, momentum, energy and entropy

Insertion of the quantities from Table 1 into the generic equations of balance (2) leads to the following specific jump conditions

$$\begin{aligned}
 0 &= \left[ \rho \left( v_i - v_{\perp s} n_i \right) \right] n_i, \\
 [t_{ai}] n_i &= \left[ \rho \left( v_a - v_{\perp s} n_a \right) \left( v_i - v_{\perp s} n_i \right) \right] n_i, \\
 [q_i] n_i &= \left[ \rho \left( u + \frac{1}{2} \left( \mathbf{v} - v_{\perp s} \mathbf{n} \right)^2 \right) \left( v_i - v_{\perp s} n_i \right) \right] n_i + \left[ t_{ia} \left( v_a - v_{\perp s} n_a \right) n_i \right], \\
 \left[ \frac{q_i}{T} \right] n_i + \left[ \rho s \left( v_i - v_{\perp s} n_i \right) \right] n_i &= \sigma_s.
 \end{aligned} \tag{3}$$

We introduce two assumptions:

- (zeroth law of thermodynamics)

The temperature is continuous across the phase boundary.

- (Coherency)

The tangential velocity  $\mathbf{v}_{\parallel}$  is continuous across the phase boundary.

The first of these conditions permits the elimination of  $[q_i] n_i$  between (3)<sub>3,4</sub> and we obtain

$$\left[ u - Ts + \frac{1}{2} \left( v_e n_e - v_{\perp s} \right)^2 \right] \rho \left( v_i - v_{\perp s} n_i \right) n_i - \left[ t_{ia} \left( v_a - v_{\perp s} n_a \right) n_i \right] = -T \sigma_s. \tag{4}$$

The second condition combined with (3)<sub>2</sub> implies that the tangential component of the stress vector  $t_{ai} n_i$  is continuous at the coherent phase boundary. Therefore (4) may be written in the form

$$\left[ \left( u - Ts + \frac{1}{2} \left( v_e n_e - v_{\perp s} \right)^2 \right) \delta_{ai} - \frac{t_{ai}}{\rho} \right] n_a n_i \rho \left( v_e n_e - v_{\perp s} \right) = -T \sigma_s. \tag{5}$$



We recall that the right hand side of (5) is non-positive and denote the mass flux  $\rho \left( v_i - v_{\perp s} n_i \right)$  per unit area of the phase boundary by  $\dot{m}$ . Thus we obtain the entropy inequality in the form

$$\left[ \left( u - Ts + \frac{1}{2} \left( v_e n_e - v_{\perp s} \right)^2 \right) \delta_{ai} - \frac{t_{ai}}{\rho} \right] n_a n_i \dot{m} \leq 0. \quad (6)$$

## 2.5 Eshelby tensor, or tensor of free enthalpy

In the manner of thermodynamics of irreversible processes we satisfy the inequality (6) by setting

$$\dot{m} = -D \left[ \left( u - Ts + \frac{1}{2} \left( v_e n_e - v_{\perp s} \right)^2 \right) \delta_{ai} - \frac{t_{ai}}{\rho} \right] n_a n_i, \quad \text{where } D \geq 0. \quad (7)$$

It is thus possible to say that the normal component of this tensor

$$g_{ai} = \left( u - Ts + \frac{1}{2} \left( v_e n_e - v_{\perp s} \right)^2 \right) \delta_{ai} - \frac{t_{ai}}{\rho}, \quad (8)$$

between the two phases is the driving force of the phase transition. Or else we may say that the normal component of this tensor is continuous across the boundary in phase equilibrium.

The tensor  $g_{ai}$  is called the Eshelby tensor, because Eshelby [2] first discovered its decisive role for the phase equilibria of inclusions in solids. Obviously for a fluid in equilibrium - where  $v_e n_e = v_{\perp s}$  holds and  $t_{ai} = -p\delta_{ai}$  - the Eshelby tensor reduces to the specific free enthalpy

$$g = u - Ts + \frac{p}{\rho} \quad \text{or, with } \frac{1}{\rho} = v: \quad g = u - Ts + pv. \quad (9)$$

And, indeed, the continuity of the free enthalpy is the condition of phase equilibrium in fluid phases as is well-known to students of thermodynamics.

In the sequel we ignore the specific kinetic energy term  $\left( v_e n_e - v_{\perp s} \right)^2$  in the Eshelby tensor. It is a non-linear term and thermodynamics of irreversible processes would drop it as a matter of course anyway.



We proceed to investigate a simple case of a bi-axially loaded solid in its melt. This is a case where the tensorial character of the Eshelby tensor makes a difference.

### 3 Phase transition between an isotropic elastic solid and its melt, - both incompressible

#### 3.1 An incompressible fluid

In an incompressible liquid we have - with  $c$  as specific heat and  $v$  as specific volume -

$$\begin{aligned} (1) \quad u_L &= u_L^R + c_L (T - T_R) = -p_R v_L + c_L (T - T_R), \\ s_L &= s_L^R + c_L \ln \frac{T}{T_R} = c_L \ln \frac{T}{T_R}. \end{aligned} \quad (10)$$

$R$  denotes a reference state with  $T_R$ ,  $p_R$ . It is often agreed that the specific values of enthalpy and entropy are set equal to zero in the reference state for *the* phase which prevails in the reference state. We take this to be the fluid phase and thus we obtain the second equations in (10)<sub>1,2</sub>. The free enthalpy reads accordingly

$$g_{Fl}(T, p) = \underbrace{c_L \left( T - T_R - T \ln \frac{T}{T_R} \right)}_{F_L(T)} + (p - p_R) v_L. \quad (11)$$

#### 3.2 An incompressible elastic solid

In the solid phase, assumed isotropic and linearly elastic, the stress-strain relation reads

$$t_{ij} = -p\delta_{ij} + 2\mu E_{ij} \quad \text{where} \quad E_{ee} = 0. \quad (12)$$



$E_{ij}$  is the strain tensor and  $\mu$  is the shear modulus. The specific values of internal energy and entropy read

$$\begin{aligned} u_S &= -r_R - p_R v_S + c_S (T - T_R) + \mu v_S E_{ij} E_{ij}, \\ s_S &= -\frac{r_R}{T_R} + c_S \ln \frac{T}{T_R}. \end{aligned} \quad (13)$$

$r_R$  is the heat of melting in the reference state and  $\mu E_{ij} E_{ij}$  is the density of elastic energy. Accordingly the Eshelby tensor reads

$$\begin{aligned} g_{ij} &= \underbrace{\left\{ c_S \left( T - T_R - T \ln \frac{T}{T_R} \right) + \frac{r_R}{T_R} (T - T_R) + \right.}_{F_S(T)} \\ &\quad \left. (p - p_R) v_L + \mu v_S E_{pq} E_{pq} \right\} \delta_{ij} - 2\mu v_S E_{ij}. \end{aligned} \quad (14)$$

### 3.3 Melting of a block of solid under biaxial loading

We consider the situation shown in Figure 2 where a block of solid is surrounded by its melt. On the top and bottom the melt exerts the pressure  $p_1$  and laterally it exerts  $p_2$ .

In the situation represented by the figure we expect the strain tensor and the stress to have the forms

$$E_{ij} = \begin{bmatrix} \varepsilon & & \\ & -\frac{1}{2}\varepsilon & \\ & & -\frac{1}{2}\varepsilon \end{bmatrix}, \quad \text{hence } t_{ij} = -p\delta_{ij} + 2\mu \begin{bmatrix} \varepsilon & & 0 \\ & -\frac{1}{2}\varepsilon & \\ 0 & & -\frac{1}{2}\varepsilon \end{bmatrix}. \quad (15)$$



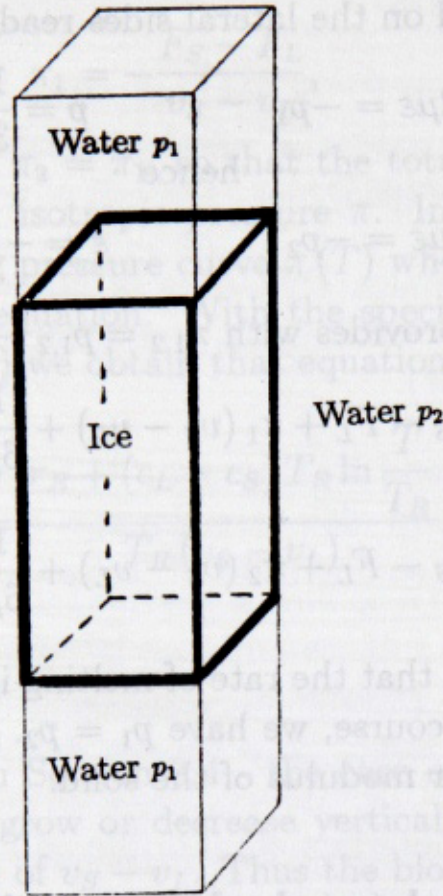


Fig. 2. Block of solid surrounded by its melt.

We have two different situations: one on the top and bottom and the other one on the lateral surfaces. Therefore we have two different melting equations of the type (7) which determine the rate of melting. Without the kinetic energy term and with (11), (14) and (15) we obtain

$$\begin{aligned} \frac{1}{D} \dot{m}_1 &= F_S - F_L + (p - p_R) v_S - (p_1 - p_R) v_L + \frac{3}{2} \mu v_S \varepsilon^2 - 2 \mu v_S \varepsilon, \\ \frac{1}{D} \dot{m}_2 &= F_S - F_L + (p - p_R) v_S - (p_2 - p_R) v_L + \frac{3}{2} \mu v_S \varepsilon^2 - 2 \mu v_S \varepsilon. \end{aligned} \quad (16)$$

Given the temperature, these conditions contain two unknowns on the right hand sides: the pressure  $p$  of the solid and the strain  $\varepsilon$ . We determine these unknowns by assuming that the dynamic equilibrium condition  $[t_{ai}] n_a n_i = 0$  prevails even though the phase equilibrium is



not yet established. By (15)<sub>2</sub> the dynamic equilibrium conditions on top and bottom and on the lateral sides read respectively

$$\begin{aligned} -p + 2\mu\varepsilon &= -p_1 & p &= \frac{1}{3}(p_1 + 2p_2) \\ \text{hence} & & & \\ -p - \mu\varepsilon &= -p_2 & \varepsilon &= -\frac{1}{3\mu}(p_1 - p_2) \end{aligned} \quad (17)$$

Insertion into (16) provides with  $\pi_{1,2} = p_{1,2} - p_R$

$$\begin{aligned} \frac{1}{D}\dot{m}_1 &= F_S - F_L + \pi_1(v_S - v_L) + \frac{1}{6\mu}v_S(\pi_1 - \pi_2)^2, \\ \frac{1}{D}\dot{m}_2 &= F_S - F_L + \pi_2(v_S - v_L) + \frac{1}{6\mu}v_S(\pi_1 - \pi_2)^2. \end{aligned} \quad (18)$$

Inspection shows that the rate of melting is different on the faces of the block unless, of course, we have  $p_1 = p_2$ . Also the rate of melting depends on the shear modulus of the solid.

### 3.4 Partial and total phase equilibrium

Let us assume that the solid block is laterally in equilibrium with its melt, so that  $\dot{m}_2 = 0$  holds. For a given pair of temperature  $T$  and pressure  $p_1$  (18)<sub>2</sub> implies that  $\pi_2$  in this case must satisfy the equation

$$\pi_2 = \pi_1 - \frac{3\mu}{v_S}(v_S - v_L) \left[ 1 - \sqrt{1 - \frac{2\{(v_S - v_L)\pi_1 + (F_S - F_L)\}}{\frac{3\mu}{v_S}(v_S - v_L)^2}} \right]. \quad (19)$$

In that case the melting occurs only on the top and bottom and its rate depends on  $p_1$  and  $T$ . We have

$$\frac{1}{D}\dot{m}_1 = \frac{3\mu}{v_S^2}(v_S - v_L)^2 \left[ 1 - \sqrt{1 - \frac{2\{(v_S - v_L)\pi_1 + (F_S - F_L)\}}{\frac{3\mu}{v_S}(v_S - v_L)^2}} \right]. \quad (20)$$



For phase equilibrium on all faces of the block we must obviously have

$$\pi_1 = -\frac{F_S - F_L}{v_S - v_L}, \quad (21)$$

and, by (19), this means  $\pi_2 = \pi_1$ , so that the total phase equilibrium can only occur under an isotropic pressure  $\pi$ . In that case equation (21) provides the melting pressure curve  $\pi(T)$  whose slope is given by the Clausius-Clapeyron equation. With the specific expressions (11), (14) of  $F_S(T)$  and  $F_L(T)$  we obtain that equation in the form

$$\frac{d\pi}{dT} = \frac{r_R + (c_L - c_S) T_R \ln \frac{T}{T_R}}{T_R (v_S - v_L)}. \quad (22)$$

### 3.5 Discussion

In the case considered in Section 3.4 - the case of lateral phase equilibrium - the block will grow or decrease vertically depending on the values of  $\pi_1$  and the sign of  $v_S - v_L$ . Thus the block may become long and thin, - needle-shaped - or it may become flat, - penny-shaped.

What we have investigated here is an extremely simple paradigm for what may happen in an alloy, when a new phase precipitates coherently from the initially prevailing phase. In such a case a stress-field is created around the precipitated inclusion by the mismatch of specific volumes of the phases. In general each point of the interface is under a different load, - just as our block is under two different loads - and therefore each point has its own melting condition of the type (7). This leads to shape changes of the inclusion which, in turn, changes the stress field, etc.

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## Appendix

We append a few remarks on the generic balance equation (1) for a quantity  $\Psi$ .

$\psi_v$  and  $\psi_s$  are the bulk and surface densities of  $\Psi$  and  $\Phi_{vi}$  and  $\Phi_s^\Delta$  are the non-convective flux densities across  $f^\pm$  and  $\partial s$  respectively.  $p_v$



and  $p_s$  are the densities of production in the bulk and on the surface. The surface is parametrized by Gaussian coordinates  $U^\Gamma$  ( $\Gamma = 1, 2$ ) such that  $x_i = x_i(U^\Gamma, t)$  is the position of the point with coordinates  $U^\Gamma$  at time  $t$ .  $\dot{\psi}_s$  is the rate of change of  $\psi_s$  for a fixed point  $U^\Gamma$ . The tangent vector on the surface is  $\tau_\Gamma^i = \partial x_i / \partial U^\Gamma$  and its gradient has tangential and normal components according to

$$\frac{\partial \tau_\Gamma^i}{\partial U^\Delta} = \Gamma_{\Gamma\Delta}^\Sigma \tau_\Sigma^i + b_{\Gamma\Lambda} n_i.$$

$\Gamma$  is called a Christoffel symbol and  $\mathbf{b}$  is the curvature tensor so that  $K_M = (1/2) b_\Delta^\Delta$  is the mean curvature.

If the surface is a material surface, a wall or a membrane (say), it is useful to consider  $U^\Gamma$  as material coordinates. But when the surface is a phase boundary, it is most appropriate to consider the points with fixed coordinates  $U^\Gamma$  as those which move normal to the surface. In that case the tangential surface velocity  $v_\Delta^s = (\partial x^i(U^\Gamma, t) / \partial t) \tau_\Delta^i$  vanishes. The semicolons in equation (1) represent covariant derivatives.

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### Ešelbi tenzor i ravnoteža faza

Pokazuje se da se Ešelbi tenzor uniformno uklapa u termodinamičku teoriju promene faze kao i teoriju ravnoteže između koherentnih faza. U ravnoteži normalna komponenta Ešelbi tenzora je neprekidna na granici faze. Jednostavan ilustrativan primer linearno elastičnog nekompresibilnog tela u ravnoteži sa svojim jednako nekompresibilnim tečnim stanjem je razmatran.