

Solid–Solid Phase–Transition as a Strain Transformation

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A solid may exhibit two crystalline structures which account for two different phases. For most of the solid–solid phase transitions standard procedures of thermodynamics are retained inadequate by metallurgists.

Basing on their viewpoint, the dominant process in the transformation of one into the other crystalline structure is due to local elastic distortions. Notions such as *strain transformation*, *self-strain*, *self-strain energy*, *coherency* are introduced and elasticity is invoked. Still however, infinitesimal elasticity can be inadequate while finite elasticity may address to new questions.

1. INTRODUCTION

Andrews isothermal pressure–volume diagrams (1869) of liquid–vapour transition and the corresponding Van der Waals mathematical model of interpretation (1873) are currently regarded as a fundamental basis for the phase–transition phenomena. Those diagrams show in evidence that a possible lack of convexity of the free energy function in one of its arguments plays a prominent role in the phenomenon. Nonetheless, the phase–transition of a solid material from one crystalline structure into a different one may highlight new aspects and address new questions. A metastable coexistence of the two crystalline structures may occur and residual stresses may be revealed in the absence of external loading. The internal stresses, in turn, can be attributed to the internal strains, or *self-strains*, having in mind the stress–strain duality which holds good in linear elasticity. Metallurgists are rather inclined to adopt the *self-strain* model since Bain proposed it, as first, in 1924, [1]. Bain’s proposal was to conceive the phase–transition as a *strain–transformation*. However, in order to envisage the possible deformation to be associated with the strain–transformation the knowledge of suitable local rotations is needed as well. We

find in the metallurgy literature that rules are prescribed for determining the local rotations [2]. Nonetheless, the prescribed rotations turn out to be finite rotations in most of the cases. The question arises then whether infinitesimal elasticity may be the appropriate framework for describing the phenomenon. Finite elasticity may be invoked but new questions emerge. For instance, the duality of the description in stresses or strains fails as one description is not equivalent to the other. Furthermore, stresses and strains have to be referred to suitable reference configurations which are unneeded in the infinitesimal elasticity theory [3]. A possible new viewpoint is expounded in the following. According to metallurgists the *self-strain* is conceived as a local distortion of a stress-free state. Hence, the strain-transformation with which it is associated, is not a deformation in the classical sense. It is rather a rearrangement of points in the reference configuration. The additional condition of *coherency* will guarantee the existence of a referential stress-free global configuration [4–6].

Based on these remarks, the Eshelby energy-momentum tensor seems to represent the proper stress tensor which governs the strain-transformation [7]. In dynamics, the inertial counterpart of the energy-momentum tensor is the *pseudomomentum*. By appealing to the balance of pseudomomentum, interesting results can be singled out for a strain transformation [8].

2. PHASE TRANSITIONS IN THERMOELASTIC SOLIDS

According to the general procedures of thermodynamics, one refers to a natural state and assumes that there exists a free energy density $W(\mathbf{C}, \vartheta)$ per unit volume of such a referential state V_R . $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, $\mathbf{F} = \text{Grad } \chi$; the mapping $\chi : V_R \rightarrow \mathcal{V}$ represents the deformation; ϑ denotes the temperature.

Consider a one-dimensional problem to start with and notice that a lack of convexity of the isothermal curves in the free energy diagram may occur just as in the Van der Waals model for fluids. By analogy, such an occurrence denotes a possible first order phase transition. A currently adopted model is the one known as the Landau-Ginzburg model [9]. According to it the free energy density is expanded in power of the interested physical quantities around the referential state. In the present case we write

$$W(\ell, \vartheta) = W_0(\vartheta) + a_1(\vartheta - \vartheta_c)\ell^2 + a_2(\vartheta - \vartheta_c)\ell^4 + a_3\ell^6 + \dots \quad (2.1)$$

where ℓ is the one-dimensional *linearized strain*. ϑ_c represents a critical temperature which is peculiar of the solid material.

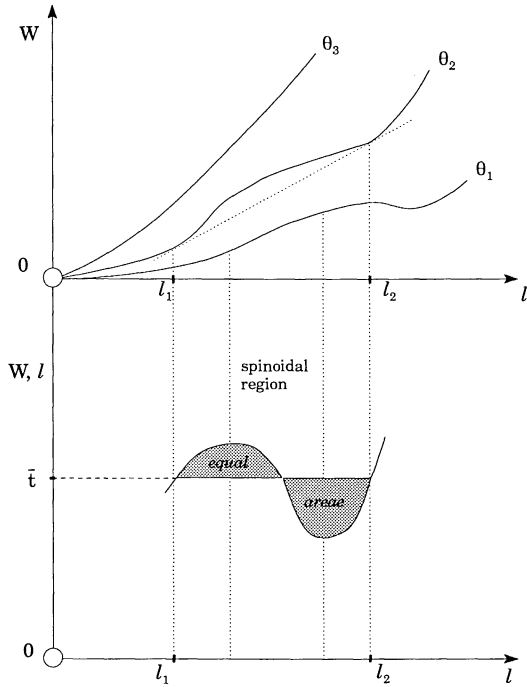


Fig. 1a and Fig. 1b

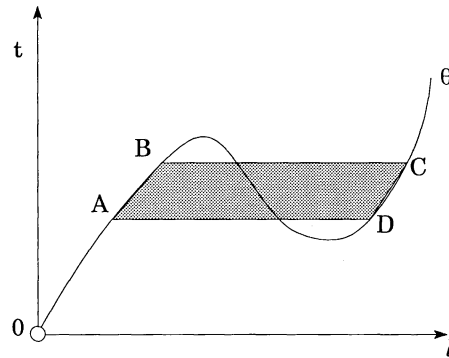


Fig. 1c

3. CONVEXIFICATION WITH THE METHOD OF THE TANGENT

The notion of linear convexification is shown in evidence in the graph of Fig. 1a through the depicted tangent to the isothermal curve.

Such a procedure is based on the fact that the mechanical and the thermodynamical equilibrium must hold true during the process. Through Fig. 1b we notice that the *method of the tangent* is equivalent to the Gibbs–Maxwell *method of equal areas* [6,7,9,10]. With reference to Fig. 1b, we also notice that both rules provide a tool for finding the unknowns \bar{t} , l_1 and l_2 . The latter quantities, in turn, individualize the phase–transition region and the two thermoelastic branches of the constitutive curve as well.

In solids however one may observe *hysteretic behaviour*. There are still two branches of the isothermal curve which account for the thermoelastic behaviour of the solid. Nonetheless, there is not a unique connection line between the two thermoelastic branches. Those lines correspond to non–reversible path while the points on the lines correspond to unstable states. For instance, the

segment AC of Fig. 1c suggests a dynamical shock-like transition.

4. THE ISOTHERMAL STRAIN-TRANSFORMATION

As each phase of the solid corresponds to a different crystalline structure Bain [1] conceived the idea that the second crystalline structure could be regarded as the first one which had been suitably strained. Such a strain-transformation or *self-strain* would provide an "intrinsic" elastic energy which is required by the phase transitions. In this respect, the *self-strain* energy would play the role of the latent heat in the classical phase transitions. Bain also suggested the proper correspondences in order that the two crystalline structures could well fit together without mismatches of the crystalline sites, namely the *coherency condition*. As a matter of fact, Bain was mainly concerned with martensitic transformations which are peculiar of steel [2]. In such transformations the two crystalline structures of interest are both cubic, and thus, they can both be described macroscopically as isotropic solids. From the microscopic viewpoint the unit lattice of one crystalline structure is body centered cubic (b.c.c.) whereas that of the other is face centered cubic (f.c.c.). The first one (α -phase) corresponds to cubic martensite and is stress free at low temperature (below room temperature for steel). The second one (γ -phase) corresponds to austenite and is stress-free at high temperature (above 800° C). Should austenite be quenched at the room temperature, it would partially transform in martensite, although the critical temperature of transformation had not been reached. A subsequent isothermal tensile or compressive loading would drive the complete transformation in martensite of the remaining part of austenite.

5. THE BAIN DEFORMATION

With reference to the figures 2a and 2b the Bain deformation reads

$$x = \sqrt{2}\alpha X; \quad y = \alpha(Y - Z); \quad z = \alpha(Y + Z). \quad (5.1)$$

Accordingly,

$$\epsilon_0 = \begin{pmatrix} \sqrt{2}\alpha - 1 & 0 & 0 \\ 0 & \alpha - 1 & 0 \\ 0 & 0 & \alpha - 1 \end{pmatrix} \quad (5.2)$$

is *candidate* to represent the *infinitesimal self-strain*. However, despite the

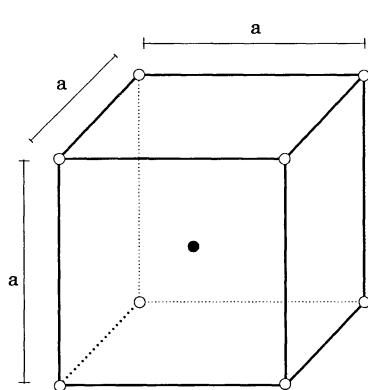


Fig. 2a

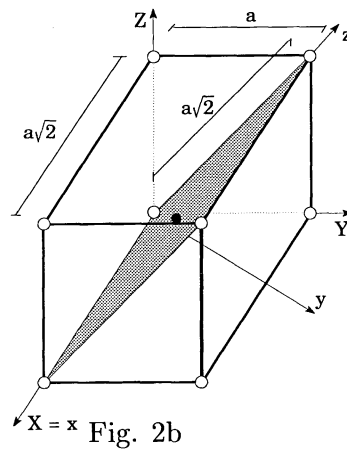


Fig. 2b

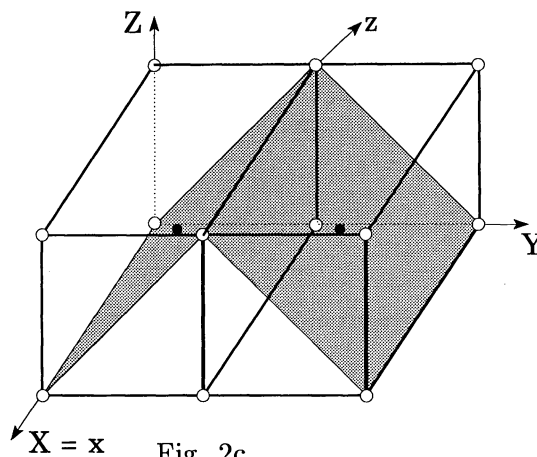


Fig. 2c

fact that the strain is possibly infinitesimal, the local rotation \mathbf{R}_0 due to the deformation (5.1) is finite. In fact one easily finds that

$$\mathbf{R}_0 = \mathbf{F}_0 \mathbf{U}_0^{-1} \quad \mathbf{U}_0^2 \equiv \mathbf{C}_0 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix} \quad (5.3)$$

namely that a finite rotation of $\pi/4$ accompanies the deformation. In addition, the finite rotation \mathbf{R}_0 remains unaltered irrespectively of the microscopic parameter α . α represents the ratio of the edges of the cubic cells. The case of $\alpha = 1$, which is represented in Fig. 2a, 2b and 2c is enlightening.

6. A FIRST APPROACH TO THE MACROSCOPIC DESCRIPTION

The *self-strain* has to be regarded as an “a priori” quantity which is provided by experimental results. In linear elasticity and under suitable assumptions, one can associate the self-strain to the residual stress and conversely. Thus, two different free energy densities correspond to the two phases, respectively. In the quadratic approximation we expand the free energy around the possibly stable states ϵ_{01} and ϵ_{02} as follows

$$W = \begin{cases} W_{01}(\vartheta) + \frac{1}{2}(\epsilon_1 - \epsilon_{01}) \cdot \mathbf{A}_1(\epsilon_1 - \epsilon_{01}) \\ W_{02}(\vartheta) + \frac{1}{2}(\epsilon_2 - \epsilon_{02}) \cdot \mathbf{A}_2(\epsilon_2 - \epsilon_{02}). \end{cases} \quad (6.1)$$

We will oversimplify the model in order to highlight the main features we are interested in. In this respect we assume that the first state is a natural one: $W_{01} \equiv 0$; $\epsilon_{01} \equiv 0$. We also assume that $\mathbf{A}_1 \equiv \mathbf{A}_2$ as we wish to disregard second order phase-transitions. Under such assumptions the *self-strain energy* is $e \equiv \frac{1}{2}\epsilon_0 \cdot \mathbf{A}\epsilon_0$. Once more we will refer to the one-dimensional case in which we recover the so-called two-parabolae model. One easily realizes that the stability of the state corresponding to ϵ_0 (the second phase) may be lost depending upon the ratio $\frac{e}{W_{02}}$.

Experimental indications on the stability of the second phase are found by a comparison with the values of the latent heat of transformation. Based on these data one realizes that the second phase is stable in many circumstances. Hence, the model of the strain-transformation is reasonably acceptable. Nonetheless, some remarks need to be made. First we notice that two linearizations occur in the two-parabolae model. The first one is *geometrical*: one global configuration is attributed to the two stable states. The second one is concerned with the constitutive form of the free energy which is assumed to be quadratic in the strain. The two-parabolae model eludes the very important geometrical aspects of the three-dimensional solid bodies: the geometrical compatibility conditions. The discussion of this point will lead to the notion of *geometrical coherence*.

7. THE FINITE ISOTHERMAL STRAIN-TRANSFORMATION

As the reference configuration V_R of the solid body might not be a natural one, one may wish to associate a natural configuration V_c with it. This can be done through the invertible map $\mathbf{P} : TV_c \rightarrow TV_R$ as follows

$$\mathbf{P}^{-1}\delta\mathbf{X} = \delta\xi, \quad \underline{\mathbf{X}} \in V_R. \quad (7.1)$$

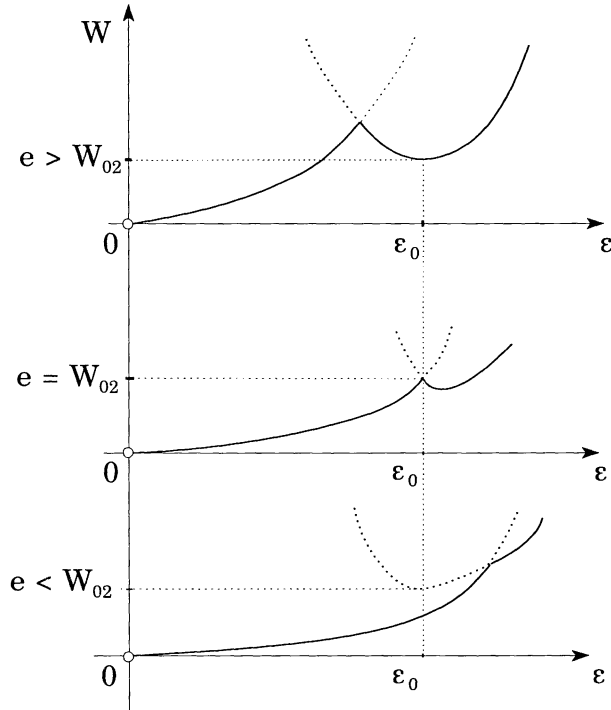


Fig. 3

\mathbf{P}^{-1} may not be integrable. Hence, V_c may not represent a global configuration but rather a collection of local configurations [5]. With reference to the model of strain-transformation, we assume that one of the two phases of the solid (say the first) represents a natural configuration. By contrast, the second phase is associated with a natural configuration V_c through \mathbf{P} . As the global energy has to be invariant with respect to changes of configurations one writes

$$W_2 \equiv W_2(\mathbf{F}, \mathbf{X}, \vartheta) \equiv J_p^{-1} \tilde{W}_2(\mathbf{FP}, \vartheta). \tag{7.2}$$

Notice that

$$\begin{aligned} \frac{\partial W_2}{\partial \mathbf{F}} &\equiv \mathbf{T}_R && \text{is the 1st Piola-Kirchhoff stress tensor,} \\ -\frac{\partial W_2}{\partial \mathbf{P}} \mathbf{P}^T &\equiv \mathbf{b} && \text{is the Eshelby stress tensor.} \end{aligned}$$

\mathbf{T}_R governs the deformation and the motion. \mathbf{b} governs the strain-transformation.

CONCLUSIONS

Based on the expounded viewpoint one is encouraged to introduce a dynamical description of the process by appealing to the *balance of pseudo-momentum* [6,8]. Within this framework the notion of *full coherency* stems naturally and interesting results can be pointed out. Some of them are known and pertain to the realm of thermodynamics [10].

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