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MECHANICS

From the propagation of phase-transition fronts to the evolution of the growth plate in long bones

Dedicated to Jüri Engelbrecht on the occasion of his 70th anniversary

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Abstract. The various methodologies exploited in the study of the propagation of phase transition fronts in crystalline substances (inert matter) are examined and compared with a view to identifying mathematical tools useful in a scientific mechanobiological approach to the critical problem of the growth of long bones in mammals.

Key words: mechanobiology, phase transition, nonlinear waves, solitons, long bones.

1. INTRODUCTION

On the one hand, the propagation of phase-transition fronts is one of the main problems in materials science [1]. On the other hand, the problem of the evolution of the growth plate at the end of long bones is identified as a critical problem in mechanobiology (cf. [2]). It was inevitable that these two apparently unrelated subject matters would somehow meet on common research lines to the benefit of the latter as applied mathematical tools developed for the former of necessity find applications in the latter. This concerns more particularly the complexity of dynamic wave phenomena involving structured or non-structured wave fronts, solitary waves, and dissipative structures. This suits the celebration of the 70th anniversary of Jüri Engelbrecht, a scientist who has devoted most of his works to various aspects of complexity and nonlinear wave propagation (cf. his book [3]). I met Jüri for the first time on an occasion already devoted to nonlinear waves (Tallinn Meeting on Nonlinear Deformation Waves, January 1978) where I presented a paper on one of my dearest research fields, that of the propagation of strongly localized nonlinear waves in any of their disguises [4]. The combined biomechanical aspect of the present work also partakes of Jüri's interests.

Of course, we must be conscious that absolutely identical schemes cannot strictly apply simultaneously to inert matter (e.g., crystals) and living matter (e.g., soft biological tissues). Straightforwardly applied analogies between these two fields may be misleading, and the inherent complexity of the evolution of physiological processes may be mistreated by our reductive simple-mindedness. There are uses and misuses of analogies. All this kept in mind, we present here some of these useful analogies after delineating the various approaches to the first problem, which they share (the Hugoniot relation) as common results and which distinguishes one from the others (dissipation or no dissipation, micro- or macrodissipation).

2. VARIOUS APPROACHES TO THE PROPAGATION OF PHASE-TRANSITION FRONTS (INERT MATTER)

In a more or less recent past we have dealt in detail with various aspects and approaches to the problem of propagation of phase-transition fronts. In doing so we have identified four types of approach, which would generally lean essentially on the background and taste of the involved scientist. We have thus:

Type-1 approach: discrete crystal lattice, condensed-matter physics;
Type-2 approach: continuum, thermomechanical engineering;
Type-3 approach: continuum, structured front, applied mathematics;
Type-4 approach: quasi-particle, theoretical physics.

2.1. Type-1 approach

The Type-1 approach concerns a *microscopic scale* (lattice dynamics) in the absence of thermodynamic irreversibility. This first scale, inspired by the Landau–Ginzburg theory, although discrete to start with, deals with nonlinear localized waves (solitonic structures: solitary waves, soliton complexes) where nonlinearity and dispersion (discreteness) are the main ingredients. This approach considers a *perfect lattice*, so that there is no dissipation and no effects of temperature are involved, except perhaps in the phase-transition parameter. Following works by Falk [5], Pouget [6], and Maugin and Cadet [7], in passing from a lattice to a continuous long-wavelength limit, this allows one to readily obtain a dynamic representation of a phase boundary (e.g, a kink) as a *solitonic structure* for a two-degrees-of-freedom, but essentially one-dimensional, system. The reason for this is that, unless one wants to study the *lateral stability* of this system, the "theorem of the flea" applies: at its scale the "flea" sees only the *first-order geometrical description* of the transition layer, hence essentially the normal direction to a layer of constant thickness. Notice that the continuum model obtained in this *long-wavelength limit* is that of a *nonlinear elastic body with first gradients of strains* taken into account but no dissipation. This long-wave limit is admissible because the transition layer between two phases, although thin (perhaps a few lattice spacings), is nonetheless large enough. Numerical simulations can be performed *directly* on the lattice. The elastic potential is non-convex in general.

To exemplify this approach, one may consider a one-dimensional (x), two-degrees-of-freedom, lattice with transverse (main effect) and longitudinal (secondary effect) displacements from the initial position. In the so-called long-wave limit where the discrete dependent variables (shear and longitudinal strains) s_n and ε_n vary slowly from one lattice site to the next and can be expanded about the reference configuration $(na, 0)$, the discrete equations yield a system of two (nondimensionalized) coupled partial in (x,t) differential equations (with an obvious notation for partial x and t derivatives), which is none other than a relatively complex system of continuum equations, where s and ε are the shear and elongation strains, γ is a coupling coefficient, and α is a nonlocality parameter. Parameters c_T and c_L are the characteristic speeds of the linear elastic system. This corresponds to stresses and energy density given by

$$\sigma_s = \overline{\sigma}_s - m_x, \quad \sigma_\varepsilon = \frac{\partial W}{\partial \varepsilon}, \quad \overline{\sigma}_s = \frac{\partial W}{\partial s}, \quad m = \frac{\partial W}{\partial s_x} \tag{1}$$

and

$$W(s,\varepsilon,s_x) = \frac{1}{2}\left(c_T^2 s^2 - \frac{1}{2}s^4 + \frac{1}{3}s^6 + c_L^2\varepsilon^2 - 2\gamma s^2\varepsilon + \alpha s_x^2\right). \tag{2}$$

Equations $(1)_{1,2}$ define the involved stresses and hyperstresses present in the balance of (physical) linear momentum for a continuum made of a nonlinear, homogeneous elastic material with strain gradients with both nonlinearity and strain gradients relating only to the *shear* deformation. As already noticed, this apparently complicated system still admits exact dynamic solutions of the *solitonic type*. A thorough discussion of the existence of solitary-wave-like solutions connecting two different or equivalent minimizers (i.e., two phases) of the potential energy was given by Maugin and Cadet [7] to whom we refer the reader. The sixth order energy (2) in s is sufficient to provide a description of all possible phase transitions between one undeformed austenitic phase and two martensitic variants of opposite shear (in 3D the potential would admit 24 variants for the martensite). A remarkable fact is that such structurally complicated solutions are shown (by computation) to satisfy the following (temperature-independent) *Hugoniot* condition between *states at infinity* (in practice, far away from the front) :

$$Hugo = [\![\overline{W}(s,\varepsilon_{\text{fixed}}) - \langle\overline{\sigma}_s\rangle s]\!] = 0, \tag{3}$$

where $\overline{\sigma}_s$ is the shear strain *without* strain-gradient effect, and $\overline{W}$ is the elastic energy with such effects similarly neglected. Obviously, gradient effects play a significant role only within the rapid transition zone that the strongly localized solution represents, while outside this zone the state is practically spatially uniform, although different on both sides of the localized front. Here we have used the following definitions for the jump and mean value of any quantity a:

$$[\![a]\!] = a(+\infty) - a(-\infty), \quad \langle a\rangle = \frac{1}{2}(a(+\infty) + a(-\infty)). \tag{4}$$

Equation (3) is typical of the *absence of dissipation* during the transition, in general a working hypothesis that is not realistic. Furthermore, it can in fact be rewritten as the celebrated *Maxwell's rule of equal areas*.

2.2. Type-2 approach

The Type-2 approach belongs to the *engineering thermomechanical* approach and relates to a *macroscopic scale*, that of engineering applications. Of necessity the progress of the phase-transition front is not only accompanied by dissipation, but it is the second law of thermodynamics that constrains or directs (in the proper sense) that progress. In this approach it is assumed at each instant of time that the thermoelastic solution is known by any means – analytical, but more often than that, numerical – on both sides of the phase-transition front considered as a singular surface Σ of vanishing thickness, so that one can compute a *driving force* acting on Σ. Further progress of Σ must not contradict the second law of thermodynamics. The latter, therefore, governs the local evolution of Σ which is generally *dissipative*, although no microscopic details are made explicit to justify the proposed expressions. The approach is *thermodynamic* and *incremental* (in total analogy with modern plasticity). All physical mechanisms responsible for the phase transformation are contained in the *phenomenological–macroscopic* relationship given by the *local criterion of progress* of Σ. Without entering details, which can be found in several papers (Maugin and Trimarco [8]; Maugin [9,10]) and considering from the outset the finite-strain framework, we remind the reader that at any regular point in the body (i.e., on both sides of Σ) we have the balance of (physical) linear momentum and the future heat equation written in the Piola–Kirchhoff form for a *heat-conducting thermoelastic material*. In general $W(\mathbf{F},\theta)$ is different on both sides of Σ , and generally non-convex in its first argument ($\mathbf{F}$ is the deformation gradient) and concave in the second one (the thermodynamic temperature θ). But while each phase is materially homogeneous, the presence of Σ is a patent mark of a loss of translational symmetry on the overall body, hence the consideration of a global material inhomogeneity. The field equation capturing this breaking of symmetry is the jump relation associated with the equation of momentum *on the material manifold*, i.e, what we have called the balance of material momentum in different works (e.g., [11]). This jump equation, together with that for entropy, governs the phase-transition phenomenon at Σ. If $\mathbf{N}$ is the unit normal to Σ oriented from the minus to the plus side, and we define the jumps and mean values at Σ by (compare to (4):

$$[\![a]\!] = a^+ - a^-, \quad \langle a\rangle = \frac{1}{2}(a^+ + a^-), \tag{5}$$

where $a^\pm$ are the uniform limits of a in approaching Σ on its two faces along $\mathbf{N}$, $\overline{\mathbf{V}}$ is the material velocity of Σ, S is the entropy density, θ is the thermodynamic temperature, $\mathbf{f}_\Sigma$ is the driving force acting on Σ, and $\mathbf{b}_S$ is the quasi-static part of the so-called *Eshelby stress tensor*, it is shown that for a coherent homothermal front we have

$$\mathbf{f}_\Sigma.\overline{\mathbf{V}} = f_\Sigma \overline{V}_N = \theta_\Sigma \sigma_\Sigma \geq 0, \tag{6}$$

and

$$\begin{aligned} f_\Sigma &= -Hugo_{PT}, \\ Hugo_{PT} &:= \mathbf{N}.\,[\![\mathbf{b}_S]\!]\,.\mathbf{N} = [\![W - \langle \mathbf{N}.\mathbf{T}\rangle \mathbf{F}.\mathbf{N}]\!]\,. \end{aligned} \tag{7}$$

If inertia is really neglected, then we have the following reduction (tr = trace):

$$Hugo_{PT} = [\![W - tr(\langle \mathbf{T}\rangle.\mathbf{F})]\!]\,. \tag{8}$$

In this canonical formalism the driving force f_Σ happens to be purely normal but it is constrained to satisfy, together with the propagation speed $\overline{V}_N$, the surface dissipation inequality indicated in the last of Eq. (6). In other words, any relationship between these two quantities must be such that this inequality be verified. This is the basis of the formulation of a *thermodynamically admissible criterion of progress* for Σ. Indeed, we should look for a relationship $\overline{V}_N = g(f_\Sigma)$ which satisfies the last of Eq. (6). Note that in a 1D approach the expression of Hugo in Eq. (8) is formally identical to the one defined in Eq. (3).

If we "force" the system evolution to be such that there is effective progress of the front at $\mathbf{X} \in \Sigma$ while there is *no* dissipation, then we must necessarily enforce the following condition

$$f_\Sigma = 0, \quad \text{i.e.} \quad Hugo_{PT} \equiv [\![W - \langle \mathbf{N}.\mathbf{T}\rangle \mathbf{F}.\mathbf{N}]\!] = 0. \tag{9}$$

On account of the fact that the temperature θ_Σ is fixed, and the thickness of the front is taken as zero, so that uniform states are reached immediately on both sides of Σ, Eq. $(9)_2$ is none other than the condition of "Maxwell" in the one-dimensional pure-shear case. Thus a macroscopic approach dear to the engineer has allowed us to obtain, in general, a more realistic (in general, dissipative) progress of the front. The Type-1 approach then appears as a "zoom" – in the nondissipative case – on the situation described in the present paragraph since the front acquires, through this zoom magnification (asymptotics), a definite, although small, thickness and a structure while rejecting the immediate vicinity of the zero-thickness front to infinities. The next approach allows one to introduce both *thickness* and *dissipation*.

2.3. Type-3 approach

The Type-3 approach is typical of *applied mathematics*. It is *mesoscopic* and considers a structured front. Here the front of phase transformation is looked upon as a mixed *viscous-dispersive* structure at a *meso* scale. This dialectical approach in which one applies macroscopic concepts at a smaller scale to obtain an improved phenomenological description is finally fruitful. This was dealt with by Truskinovsky [12] to whom we refer for details. We therefore consider a one-dimensional model (along the normal to the structured front – "theorem of the flea") and we envisage a *competition* between viscosity (i.e., a simple case of dissipation) and some *weak nonlocality* accounted for through a strain-gradient theory (compare the Type-1 approach). The critical nondimensional parameter that compares these two effects is defined by

$$\omega = \eta/\sqrt{\varepsilon}, \tag{10}$$

where η is the viscosity and $\varepsilon \approx L^2$ is the nonlocality parameter (size effect). Progressive-wave solutions $u = u(\xi = x - \overline{V}_N t)$ of the continuous system that relate two minimizers (uniform solutions at infinities that minimize $\overline{W}$) over a distance of the order $\delta = \sqrt{\varepsilon}$ are discussed in terms of this parameter. The mathematical problem reduces to a *nonlinear eigenvalue problem* of which the specification of the points of the discrete spectrum constitutes the looked for *kinetic relation* $\overline{V}_N = g(f;\varepsilon)$, where $f = \overline{\sigma} - \overline{\sigma}(+\infty)$ plays the role of the *driving force*. As a matter of fact, the speed of propagation $\overline{V}_N$ satisfies the *Rankine–Hugoniot equation* $\overline{V}_N^2 = [\![\overline{\sigma}]\!] / [\![s]\!]$, where strain gradients and viscosity play no role and the jumps are taken between asymptotic values at infinity (cf. Eq. (4)). The evolution obtained for the kinetic law is a strongly nonlinear function and evolves with the value of the parameter ω.

2.3. Type-4 approach

The Type-4 approach is one that would suit a *theoretical physicist*. Exploiting the formalism of field theory, one associates with the strongly localized nonlinear solutions such as those envisaged in the Type-1 approach the dynamics of a *quasi-particle* that gathers in its definition of mass and the driving force acting or not acting on it (then in inertial motion representing the stationary motion of the structured but nondissipative transition front viewed as a "massive" object) the type of involved transition (i.e., particular solutions to the PDEs). This was studied in some detail by Maugin and Christov [13] on the basis of soliton-like solutions of the Type-1 approach, which yielded some strange "point dynamics" depending on the original system of governing partial differential equations. Typically, one obtains a motion equation of the form

$$\frac{d}{dt}\left(M(V)V\right) = [\![F]\!] , \tag{11}$$

where $M(V)$ is the velocity-dependent "mass" of the said quasi-particle, and inertial motion requires the vanishing of the right-hand side, here written symbolically as the difference ("jump") between the values of a driving force between plus and minus infinity, again defined in terms of the value of the "Eshelby stress" at infinities. This is a hidden form of the *Hugoniot condition* as in the absence of dissipation and of any external forcing on the motion of the quasi-particle. However, the formulation (11), esoteric as it may look to many engineers, is one that allows for the study of the perturbation of the inertial motion of the "phase-transition structure" by offering a direct perturbation scheme in which one looks for the time modulation of the motion (e.g., an acceleration or a slowdown). Any "obstacle" (viscous zone, foreign object, etc.) met on the path of the quasi-particle will materialize in a non-vanishing right-hand side in Eq. (11). Because of their association with wave processes, we like to refer to the relevant quasi-particles as "*wavicles*" [13]. As a partial conclusion of this section, we note that the various approaches considered here have in common the notion of Hugoniot condition or a relaxed form of it when the Hugoniot functional, not set equal to zero, itself produces dissipation. The various approaches may also be pictured as in Fig. 1.

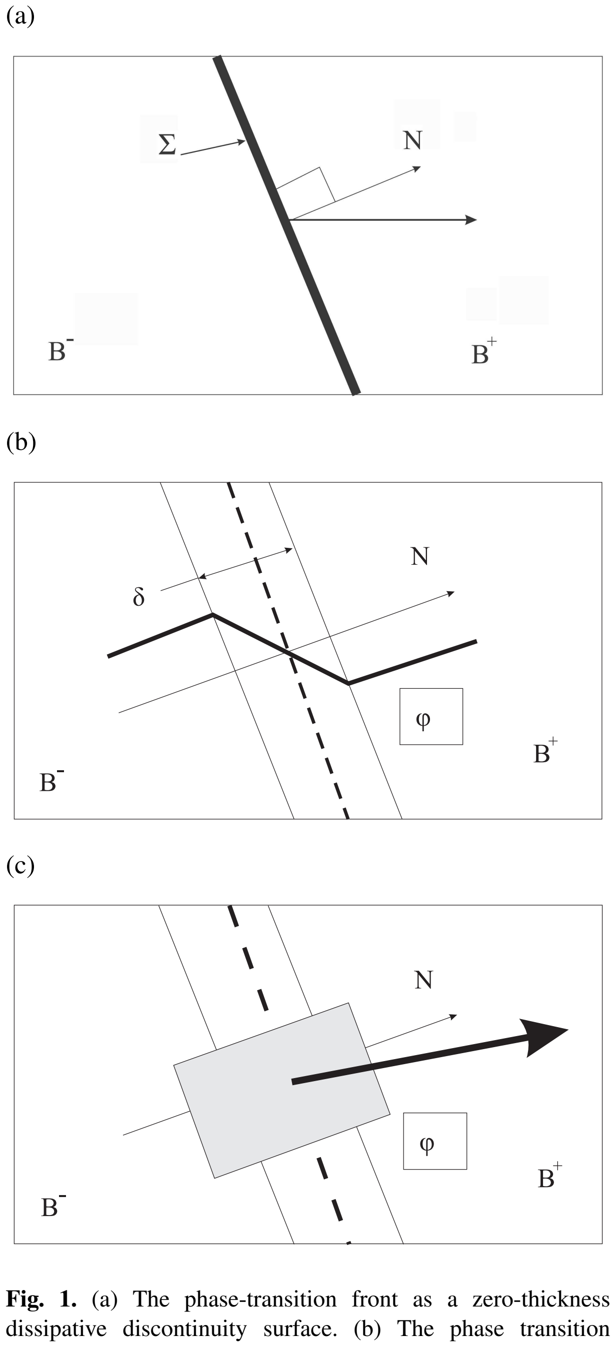

Fig. 1. (a) The phase-transition front as a zero-thickness dissipative discontinuity surface. (b) The phase transition seen as a relatively thick transition zone presenting a local dissipation, and possibly a microstructure (e.g., gradient type or Cosserat type; the linear variation is just an illustration conveniently defining the thickness). (c) The phase-transition front seen locally as a quasi-particle moving with a dynamics deduced from the localized solution of the PDEs.

3. THERMODYNAMICALLY BASED CONTINUOUS AUTOMATON

Recently, in order to treat numerically the progress of phase-transition fronts in thermoelasticity, Berezovski and I [14] introduced a numerical strategy which, while based on the thermodynamic, no-thickness singular surface such as the Type-2 (engineering) approach of the previous section, allows for the automatic application of the criterion of transformation during the progression, providing simultaneously a more reasonable (nonlinear) kinetic law, which is here part of the solution. This is a performing finite-volume method (FVM) adapted so as to include the balance of material momentum and its jump at the phase boundary. This is all the more appropriate that the fixed FVM cells thus considered may also be viewed as the elementary blocks of a thermodynamics of so-called *discrete systems* in the manner of Schottky (cf. Muschik [15]). In this thermodynamics the state in one discrete system (e.g., one of the computing cells) is defined in terms of its environment which may or may not be in thermodynamic equilibrium. *Contact thermodynamic quantities* (e.g., contact temperature, contact stresses, contact velocity) are introduced to characterize the state of the discrete system (in fact defined at the boundary surface of a cell in the FVM). This idea of making a cell's state depend on that of its neighbours is tantamount to introducing a strategy for the propagation of the thermodynamic state. Although discretization here is based on continuous balance laws, we may refer to this method as that of *continuous cellular automata*. The strategy referred to above is essential in the case of the dynamics of a *phase-transition front*. In this scheme, all thermomechanical balance laws are expressed for each cell, and the bulk quantities within each cell are related to the contact ones through the thermodynamics of discrete systems. Thereby a high-performance wave-propagation algorithm is exploited – combining Lax–Wendroff and Godunov's ideas (Berezovski and Maugin [14]) – that yields extremely good results in the simulation of the rapid progression of sharp wave fronts in 2D thermoelasticity under the external action of an applied stress shock. The thermodynamic justification of the scheme and technical details are given in a recent book [16]. The kinetic relation obtained by computing separately the driving force and the velocity of the front compares favourably with that deduced from the mesoscopic approach recalled in the previous section.

4. MECHANOBIOLOGICAL PROBLEM OF THE GROWTH PLATE EVOLUTION (SOFT TISSUES)

Some physiological problems involving mechanics may look like problems dealing with phase-transition fronts. This is the case of the growth of long bones under the influence of mechanical factors. Here the main phenomenon is the growth at the so-called growth plate that connects the metaphyseal bone and the epiphyseal bone [2]. This transition zone, which may be called the "chondro-osseous junction" (from bone to cartilage), has a long-time stationary motion occurring with a competition between proliferation and hypertrophy of chondrocytes and the ossification process. In spite of the complexity and multiplicity of processes involved in the activation of the different behaviours of the chondrocytes, the growth plate considered may first be viewed as a singular surface of a vanishingly small thickness in steady motion (during the lengthening of the bone, which takes years) that is governed by a kinetic law such as

$$V_\Sigma = K\tau_N, \quad K > 0, \tag{12}$$

where ($\mathbf{b}_s$ is the quasi-static par of the Eshelby stress and Σ connects two regions of differing elasticity, bone and cartilage; the μ's are chemical potentials)

$$\tau_N = -\mathbf{N}.\,[\![\mathbf{b}_s]\!]\,.\mathbf{N} = -(\mu_{\text{bone}} - \mu_{\text{cart}}), \quad \mathbf{b}_s = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}, \tag{13}$$

so that the local dissipation inequality $V_\Sigma f_\Sigma > 0$, $f_\Sigma + \tau_N = 0$, is satisfied. Bone and cartilage have different (nonlinear) elastic potentials. $\mathbf{N}$ is the unit normal to the growth plate and both displacement and traction are continuous at Σ. The stability of the motion (12) can be studied. It is found that compression decreases the interface rate while traction favours the lengthening of the bone (increase in V_Σ) as experimentally observed (cf. [17]).

It is clear that this type of approach is identical to the Type-2 approach of Section 2. However, it is easily conceived that the problem at hand is much less cartoonesque than that, since (i) here only mechanical effects are taken into account, (ii) the real growth plate has a definite thickness in which complicated rearrangements take place with an obviously present microstructure, and (iii) the ultimate fate of the growth plate is to close leaving only a fine print in the form of a trace at the end of its evolution – a possible cause of further problems such as decohesion, fracture – after consuming all its available energy and that of the nutriments (no more orders from hormones) when growth is completed in adulthood. Accordingly, a possible complexification of the modelling of the evolution of the growth plate can be considered as in Fig. 2. There, Part (b) corresponds to the Type-2 approach as discussed above. Part (c) would consider a finite thickness with a transition zone that includes a (not necessarily dissipative) microstructure and perhaps gradients in some of the physical properties (such as in the elasticity coefficients, as demonstrated by experimental data obtained on the long bones of rabbits [18]). This will provide a description closer to the Type-1 approach of Section 2. Finally, with a thickness diminishing in time and the closing of the growth plate we are in a situation which recalls the motion of a nonsymmetric dissipative structure or the time evolution of a quasi-particle terminating after a long time.

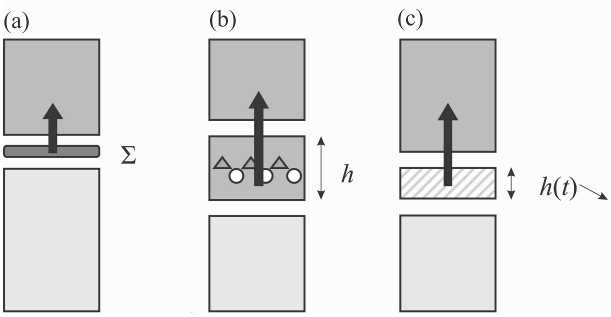

Fig. 2. Schematization of the progress of the growth plate: (a) zero thickness interface between two elastic materials (bone and cartilage); (b) microstructured interface with internal structural rearrangements; (c) time-evolving structure terminating with a zero thickness.

The completion of the three schemes represents a long-time programme of research.

5. CONCLUSION

We have first perused the various schemes that can be applied to describe the more or less dissipative and stationary motion of phase-transition fronts in inert materials (crystals). Then a rather rapid description of the problem posed by the long-time evolution of the growth plate in long bones of mammals allowed us to pinpoint the many traits in common with various aspects of the first problem and the necessary appearance of commonly shared notions such as that of the Eshelby stress. However, the first intuitive approach is purely mechanical and lacks physiological aspects that require that the more realistic formulation should include some diffusive effects related to nutriments since the system considered cannot be an isolated one; it is open from the point of view of thermodynamics. The type of approach delineated and corresponding to parts (b) and (c) in Fig. 2 is closer to the more involved approaches to the propagation of phase fronts. In addition, some of the theories advanced for the growth of soft tissues (e.g., [19]) may be involved that combine with more recent ideas such as introduced in the work of, among others, Ambrosi and Guillou [20]. This shows that the analogy with what happens in inert matter may be useful but it will not be sufficient in a more inclusive scientific approach to our mechanobiological problem.

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Faasiülemineku frontide levilt kasvuvööndi evolutsioonini pikkades luudes

Gérard A. Maugin

On vaadeldud ja võrreldud erinevaid metoodikaid, mida on kasutatud faasiülemineku frontide levi uurimisel kristallsetes ainetes (inertsetes materjalides) eesmärgiga kindlaks määrata efektiivsed matemaatilised vahendid, mis võivad osutuda kasulikuks imetajate pikkade luude kasvu kriitilise probleemi teaduslikul mehaanilis-bioloogilisel käsitlemisel.