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The average conformation tensor of inter-atomic bonds as an alternative state variable to the strain tensor: definition and first application – the case of nanoelasticity

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Most of the mechanical models for solid state materials are in a methodological framework where a strain tensor, whatever it is, is considered as a thermodynamic state variable. As a consequence, the Cauchy stress tensor is expressed as a function of a strain tensor—and, in many cases, of one or more other state variables, such as the temperature. Such a choice for the kinematic state variable is clearly relevant in the case of infinitesimal or finite elasticity. However, one can ask whether an alternative state variable could not be considered. In the case of finite elastoplasticity, the choice of a strain tensor as the basic, kinematic state variable is not totally without issue, in particular in relation to the physical meaning of the internal state variable describing the permanent strains. In any case, this paper proposes an alternative to the strain tensor as a state variable, which is not based on the deformation (Lagrangian) gradient: the average conformation tensor of inter-atomic bonds. The purpose, however, is restricted to (1) a particular type of materials, namely the pure substances (copper or aluminium, for instance), (2) the nanoscale, and (3) the case of elasticity. The very simple case of two atoms of a pure substance in the solid state is first considered. It is shown that the kinematics of the inter-atomic bond can be characterized by a so called "conformation" tensor, and that the tensorial internal force acting on it can be immediately deduced from a single scalar function, depending only on the conformation tensor: the state potential of free energy (or interaction potential). Using an averaging procedure, these notions are then extended to a finite set of atoms, namely an atom and its first neighbours, which can be seen as the "unit cell" of a pure substance in the solid state considered as a discrete medium. They are also transposed to the Continuum case, where an expression of the Cauchy stress tensor is proposed as the first derivative of a state potential of density (per unit mass) of average free energy of inter-atomic bonds, which is an explicit function of the average conformation tensor of inter-atomic bonds. By applying a standard procedure in Continuum Thermodynamics, it is then shown that the objective part of the material derivative of this new state variable, at least in the case when the pure substance can be considered as an elastic medium, is equal to the symmetric part of the Eulerian velocity gradient, that is the rate of deformation tensor. In the case of uniaxial tension, a simple relationship is eventually set out between the average conformation tensor and a strain tensor, which is correctly approximated by the usual infinitesimal strain tensor as long as the conformation variations (from an initial state of conformation) are "small". From this latter result, and assuming an elastic behavior, a simple expression for the state potential of density of average free energy is inferred, showing great similarities with—but not equivalent to—the classical model of isotropic, linear elasticity (Hooke's law).

Keywords: solid state, inter-atomic bonds, conformation tensor, continuum mechanics, Cauchy stress tensor, continuum thermodynamics, uniaxial tension, elasticity model

1 Introduction

Any mechanical behavior model for a solid state material is defined by a set of constitutive equations, one of these equations generally linking the Cauchy stress tensor $\boldsymbol{\sigma}$ to a strain tensor $\boldsymbol{S}$ and, if necessary, to so called internal variables (Coleman and Owen 1974), such as a plastic strain tensor or a damage variable. In most cases—and for the constitutive equations to be thermodynamically admissible—the stress-strain equation is obtained by differentiating a state potential of density (per unit mass) of Helmholtz free energy ψ, namely

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{S}} \tag{1}$$

where ρ is the density of the material. Thus, like the eventual internal variables and, in thermomechanics, the temperature, a strain tensor $\boldsymbol{S}$ is one of the variables on which ψ depends, in other words, it is a state variable. Let us first recall that the tensor field of current strains $\boldsymbol{S}(\boldsymbol{x}_t, t)$ links the current configuration (i.e. the set of position vectors of the particles of a solid at current time t: $\Omega_t = \{\boldsymbol{x}_t\} \in \mathbb{R}^3$) to a reference one ($\Omega_r = \{\boldsymbol{x}_r\} \in \mathbb{R}^3$), most often equal to the initial configuration. More precisely, and at the local level, i.e. at any point of the solid, denoting by $\boldsymbol{\varphi}$ the Lagrangian description of the solid motion (such that $\boldsymbol{x}_t = \boldsymbol{\varphi}(\boldsymbol{x}_r, t)$), $\boldsymbol{S}$ is built from the gradient of this description, $\boldsymbol{T} = \mathbf{grad}_L\, \boldsymbol{\varphi}$, usually called the *local deformation gradient*. In other words, a strain tensor, by construction, is irreducibly linked to a Lagrangian gradient, which itself links Ω_t to Ω_r, whatever the evolution of the configuration between t_r and t.

Since the pioneer work of Eringen (1980), among others, this way of building a mechanical model has been widely and successfully used. Most of the proven mechanical models are built in this way. They are sometimes called—at least in the isotropic, elastic case, for which $\boldsymbol{S}$ is the only state variable to be taken into account—*hyper-elastic models* to underline that the $\boldsymbol{\sigma} - \boldsymbol{S}$ relationship derives from a state potential (Adkins 1961; Fu and Ogden 2001). The important point that must be emphasized is that all these models are actually based on an implicit assumption, namely that the only kinematic variable which can be associated with the Cauchy stress tensor is a strain tensor—or, in the elastoplastic case, an elastic part of a strain tensor. The fact is that the multitude of experimental results concerning the mechanical behavior of materials in the solid state does not disprove this assumption, where some component (in a prescribed basis) of the stress tensor undoubtedly depends on some component of a strain tensor. It is also true that the numerical simulations based on mechanical models obeying Equation (1) most often lead to physically relevant results. However, neither the experiments nor the numerical simulations definitely prove that a strain tensor $\boldsymbol{S}$ is the first and only kinematic variable which can be associated with $\boldsymbol{\sigma}$. At the very least, the question can be asked about the existence of an alternative kinematic variable. Although it seems without much interest in the elastic case, the question of whether an alternative to a strain tensor $\boldsymbol{S}$ could be used to express the stress tensor $\boldsymbol{\sigma}$ is therefore not without interest.

The same question is both relevant and interesting when mechanical models more advanced than elasticity models are considered, where, in addition to $\boldsymbol{S}$, other state variables (the internal variables) have to be taken into account. Such models are clearly outside the scope of this study, which is only devoted to elasticity. It is however interesting to mention them, but only in this introduction, because they confirm the interest of looking for an alternative kinematic variable to a strain tensor. The elastoplasticity models are well known examples of such models. In the presence of finite strains, elastoplasticity models are generally based on the assumption that the deformation (Lagrangian) gradient tensor $\boldsymbol{T}$ must follow a multiplicative decomposition into an elastic part $\boldsymbol{T}^e$ and a plastic part $\boldsymbol{T}^p$. In the vast majority of cases, the decomposition $\boldsymbol{T} = \boldsymbol{T}^e \cdot \boldsymbol{T}^p$ is selected (Mandel 1972; Asaro 1983; Boyce et al. 1989). However, it has to be said that this choice is never clearly justified, either kinematically or physically. Moreover, this way of decomposing $\boldsymbol{T}$ assumes the existence of a so-called intermediate configuration of the considered solid, which acts as a reference configuration for the calculation of $\boldsymbol{T}^e$.

Nevertheless, when the initial (reference) and current configurations are pure geometrical and kinematical concepts, the intermediate configuration can be defined only on the basis of a condition on the internal forces, namely that the stress field vanishes, at least locally. The definition of the intermediate configuration is therefore constrained by the mechanical model. In other words, the intermediate configuration for a given model is not the same as that for another model, when the real configurations—initial and current—are always the same, irrespective of the model. Moreover, apart from some very particular and simple cases, like that of the uniaxial tension of a laboratory specimen, the intermediate configuration cannot be observed: it is fictitious and, consequently, physically questionable. It is nevertheless from this ill-defined concept that a plastic deformation tensor $\boldsymbol{S}^p$ and an elastic deformation tensor $\boldsymbol{S}^e$ are proposed. As for the elastoplasticity models based on an additive decomposition of the rate of deformation tensor $\boldsymbol{D}$ in an elastic part $\boldsymbol{D}^e$ and a plastic part $\boldsymbol{D}^p$ (Rice 1971), they purely and simply ignore the issue of how the elastic and plastic strains might be described, which does not make it easy to understand their physical meaning.

At best, these last remarks, linked to the previous ones on the intermediate configuration, leave open the question of the physical meaning of $\boldsymbol{S}^e$ and $\boldsymbol{S}^p$. At worst, they sow doubt on their physical relevance. At the very least, this calls for considering that the choice of the deformation (Lagrangian) gradient tensor $\boldsymbol{T}$ as the basic, kinematical quantity, from which all the other kinematical quantities are deduced, and, in the first place, the strain tensors, raises some difficult, if not insoluble, issues. In any case, the present paper deals with the problem of the existence of a state variable—denoted by $\boldsymbol{\Gamma}$ in the continuous case—as an alternative to a strain tensor $\boldsymbol{S}$ and, more generally, without any connection with the Lagrangian gradient of some vector field. Formally, and due to the fact that this problem is closely linked to that of the definition of the Cauchy stress tensor $\boldsymbol{\sigma}$, the main question asked in this paper is the following one:

$$\text{does } \boldsymbol{\Gamma} \neq \boldsymbol{S} \text{ exist and does } \Upsilon(\boldsymbol{\Gamma}, \ldots) \text{ exist such that } \boldsymbol{\sigma} = \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}}? \tag{2}$$

where Υ denotes the state potential of the Helmholtz free energy density (per unit mass), and where the state variable $\boldsymbol{\Gamma}$, if it exists, must be physically relevant and, especially, objective (Eringen 1980; Murdoch 2003; Liu 2004). It should be mentioned that, beyond the above usual mechanical continuum approaches, other works exist where the problem of defining the Cauchy stress tensor $\boldsymbol{\sigma}$ in terms of quantities other than a strain tensor is addressed. One can quote (Kuzkin et al. 2015) where $\boldsymbol{\sigma}$ is expressed in terms of averaged interparticle distances and forces. In that paper, the solids are indeed discrete. The approach followed there and the present approach have a point in common where the basic kinematic quantity, the conformation tensor, is first defined in the discrete case. However, their purpose is not exactly the same: while the emphasis is put on the definition of $\boldsymbol{\sigma}$ from the interparticle forces in (Kuzkin et al. 2015), the Cauchy stress tensor is defined in the present study only in the continuous case, and after the notion of conformation—initially introduced in the discrete case—has been transposed to the continuous case, under precisely defined conditions.

For the sake of enhancement of the main new ideas, the question asked in Equation (2) is applied only to pure substances in the solid state, in the restricted sense of substances made up of only one type of atom, and not only one type of molecules. Metallic crystals are a good example of pure substance, in which defects, punctual or linear (dislocations), can exist. Although it will be only illustrated for perfect defect-free crystals in this study, the notion of conformation remains valid for crystals with defects, it is important to underline it. Moreover, the present study is limited to the elastic case (in the case of a crystal with defects, it must be then assumed that they are in constant number and, for dislocations at least, immobile). Although the issues linked to the usual way of modeling the elastoplastic strains are one of the reasons to look for an alternative to a strain tensor as a state variable, it is indeed necessary to demonstrate that an alternative variable to $\boldsymbol{S}$ can be found in elasticity since, in most of the materials, the mechanical behavior is first elastic before becoming, possibly, elastoplastic. Another important limitation is imposed to the purpose of this study. It relates to the spatial scale at which $\boldsymbol{\Gamma}$ is defined. As will be seen, the elementary variable from which $\boldsymbol{\Gamma}$ is deduced is defined for two atoms of a pure substance in the solid state. As a consequence, a clear physical meaning can be given to this new state variable only at the atomic scale, and the field described by $\boldsymbol{\Gamma}$ is really relevant only at the nanoscale—that of a grain in a metallic material, for instance. No micro-macro methods will be used in the present paper to investigate the physical meaning of the conformation tensor at larger scales. By contrast, an equivalent continuous medium (in the sense of an equivalence of energy, in the present case) will be associated to the real material where the conformation field, observed at the nanoscale, is discrete.

The paper is organized as follows. Two atoms of a pure substance in the solid state, that is to say linked by an inter-atomic bond, are considered in Section 2, in order to precisely define the basic kinematical and force-like quantities, namely, the conformation tensor of the inter-atomic bond and the associated, internal force tensor. The discrete modeling of a "unit cell" defined by an atom and its first neighbours is addressed in Section 3, where an average conformation tensor is defined, with a clear geometrical interpretation, as well as a tensor of average internal forces. Section 4 is devoted to the Continuum description of a pure substance in the solid state, where a continuous, quasi-uniform field of average conformation is first defined. As a direct consequence of the fact that the energy of the (real) discrete unit cell and that of the (fictitious) continuous one are equal, an average internal forces tensor (per unit mass) is next proposed. Directly linked to the latter, a definition is finally proposed for the Cauchy stress tensor. The quantities defined in Section 4 are considered from a thermodynamic point of view in Section 5. An expression is then given for the objective part of the material derivative of the average conformation tensor, which turns out to be the only possible one when the considered pure substance has an elastic behavior. The uniaxial tension is examined in Section 6, for which a relationship is easily established between the average conformation tensor and a strain tensor. The particular case of "small", elastic conformation variations (with respect to an initial state of conformation) is also discussed. From it, an expression for the state potential of the density of free energy is inferred, which shows clear similarities with—but is not equivalent to—that defining the classical model of isotropic, linear elasticity (Hooke's law).

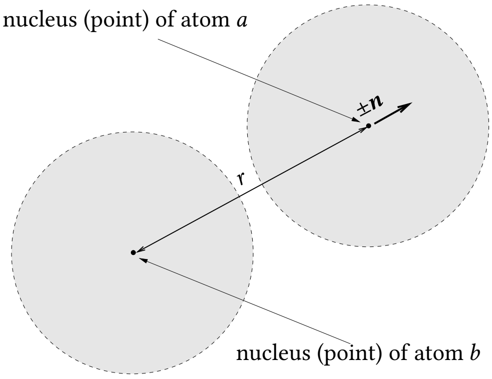
Note finally that all the arguments, hypotheses and equations detailed in this study concern a "frozen" state of a pure substance in the solid state, observed at the generic time t. In other words, the thermal and viscid effects are not taken into account. As a consequence, the thermodynamic concepts of internal energy and Helmholtz free energy are equivalent. The latter will be systematically used in all this paper.

2 Inter-atomic bond conformation tensor and internal force tensor

Let a and b be two atoms of a pure substance in the solid state, that is to say, two atoms linked by a so-called "inter-atomic bond" (e.g., a metallic bond). In this section, these two atoms are assimilated to an isolated system, in the thermodynamic sense of the word. They are therefore assumed to have no interaction of any kind with the other atoms of the pure substance that surround them. On the other hand, they do interact with each other, a force resulting from this interaction.

The characteristic size of these atoms is given by the Bohr radius, which is approximately 5×10^{-2} nm, when the radius of an atomic nucleus is approximately 5×10^{-7} nm: at the atomic scale, the nuclei can be considered as points. Furthermore, the mass of a nucleon is approximately 10^{-27} kg when that of an electron is approximately 10^{-30} kg: the mass of an atom is mainly concentrated in its nucleus. The distance between the nuclei is denoted by r—which has the same value for all the observers in classical physics—and the unit vector of the direction defined by the nuclei, by $\pm\boldsymbol{n}$, see Figure 1. Both these quantities are objective, and their product, $\pm r\boldsymbol{n}$, is nothing more than the vector of the relative position of the atomic nuclei. The length of the bond when no force is applied can be considered as a characteristic length, denoted by r_r (depending on the temperature, which however will not be taken into account in this study, where all thermal effects are neglected). Then, the normalized length of the inter-atomic bond—or, equivalently, the

Figure 1 2D representation of two atoms a and b of a pure substance in the solid state and of the inter-atomic bond linking a and b—the scale is thus approximately 10^{-1} nm. The mass of each atom is mainly concentrated in its nucleus, which is considered as a point. The distance between the nuclei is r and the unit vector of the direction defined by the nuclei is $\pm\boldsymbol{n}$. The dashed circles provide a simplistic image of the electron clouds.



normalized distance between the two nuclei—is defined by

$$\bar{r} = r/r_r. \tag{3}$$

Since r and r_r are objective quantities, so is $\bar{r}$. The problem of the non-uniqueness of the unit vector of the direction defined by the two nuclei, $\pm\boldsymbol{n}$, is solved by considering the second-order tensor

$$\boldsymbol{N} = \boldsymbol{n} \otimes \boldsymbol{n} = (-\boldsymbol{n}) \otimes (-\boldsymbol{n}). \tag{4}$$

As defined by Equation (4), $\boldsymbol{N}$ is a symmetric, positive-definite tensor. Its first three invariants are not independent since

$$\operatorname{Tr} \boldsymbol{N} = \operatorname{Tr} \boldsymbol{N} \cdot \boldsymbol{N} = \operatorname{Tr} \boldsymbol{N} \cdot \boldsymbol{N} \cdot \boldsymbol{N} = 1. \tag{5}$$

In other words, $\boldsymbol{N}$ is a uniaxial tensor with 1 as sole non-zero eigenvalue. The conformation tensor[1] of the inter-atomic bond is then defined by

$$\boldsymbol{C} = \ln(\bar{r})\boldsymbol{N}. \tag{6}$$

The only non-zero eigenvalue of the symmetric tensor $\boldsymbol{C}$ defined by Equation (6) is $\ln(\bar{r})$. In other words, $\boldsymbol{C}$ is a uniaxial tensor. Since it is defined as the product of two objective quantities, it is also an objective quantity.

The energy of the inter-atomic bond linking atom a and atom b is then classically characterized by a state potential $p(r) = q(\bar{r}(r))$ commonly called *interaction potential*—a pair potential, in this case, since the system under consideration reduces to two atoms. No particular expression is given to $p(r)$ in this study. It should just be noted that the minimum of this state potential is obtained for $\bar{r} = 1$, that is, following Equation (3), $r = r_r$. In the same classical way, the algebraic value of the internal force undergone by the atoms is directly given by the first derivative of the state potential

$$f = p'(r) = \frac{1}{r_r} q'(\bar{r}) \tag{7}$$

since $\bar{r} = r/r_r$, see Equation (3). In Equation (7), p' (resp. q') denotes the first derivative of p (resp. of q). It will be conventionally assumed in the study that $f > 0$ (resp. $f < 0$) when the internal force is a tensile one (resp. a compressive one). Furthermore, the direction of the internal force is that defined by the two atomic nuclei, $\pm\boldsymbol{n}$. Hence, the internal force vector is given by $\boldsymbol{f} = \pm f\boldsymbol{n}$. Like the vector of the relative position of the two nuclei, $\pm r\boldsymbol{n}$, $\boldsymbol{f}$ is an objective quantity.

Another expression for the internal force can be proposed, which will make it possible to once again overcome the problem of the non-uniqueness of the unit vector of the direction defined by the two nuclei. The state potential is first rewritten as a function $u(\boldsymbol{C})$. For the value of this function for a given conformation tensor $\boldsymbol{C}$ to be an objective quantity, the state potential u must depend only on the invariants of $\boldsymbol{C}$, which are linked, as previously mentioned. The square of the Euclidean norm of the conformation tensor, $\boldsymbol{C} : \boldsymbol{C} = \ln^2(\bar{r})$, is then considered as the only variable on which u depends. Obviously, the state of free energy of the inter-atomic bond is the same whether the state potential of free energy is expressed as a function of r or $\bar{r}$ or $\boldsymbol{C}$. Thus, the relation

$$u(\boldsymbol{C} : \boldsymbol{C}) = q(\bar{r}) = p(r(\bar{r})) \tag{8}$$

is necessarily verified. Given that

$$2\frac{\ln(\bar{r})}{\bar{r}} u' = r_r p' = q' = r_r f \tag{9}$$

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[1] In chemistry, the word “conformation” refers to the spatial arrangement of atoms, linked by inter-atomic bonds, in a given molecule. However, as far as the author is aware, the chemists do not give a tensorial representation to the conformation.

where u' denotes the first derivative of u, and given also that, in agreement with Equation (6)

$$\frac{\partial u}{\partial C} = u' \frac{\partial\,(C : C)}{\partial C} = 2u'C = 2\ln(\bar{r})u'\boldsymbol{N}, \tag{10}$$

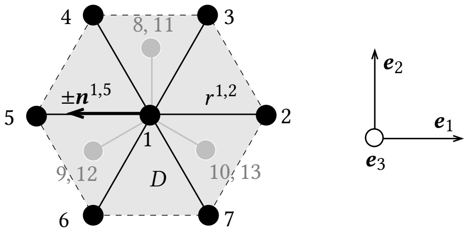
the following internal force tensor can then be defined, according to Equation (9):

$$\boldsymbol{F} = \frac{1}{r}\frac{\partial u}{\partial C} = f\boldsymbol{N}. \tag{11}$$

Indeed, thus defined, the symmetric tensor $\boldsymbol{F}$ has a single non-zero eigenvalue, $p'(r)$, which is the algebraic value f of the internal force, see Equation (7). Note also that all the quantities appearing on the right hand side of Equation (11) are objective. As a consequence, $\boldsymbol{F}$ is an objective quantity.

3 Average conformation tensor of inter-atomic bonds and average internal forces tensor: Discrete case

Any atom of a pure substance has an inter-atomic bond with some of its neighbours, the first ones but also the second if not the third ones, the fourth... However, the interactions between an atom and its first neighbours are clearly dominant. In any case, the latter are the only ones which will be considered subsequently. For metallic materials, at least, this restriction of the range of interactions allows to consider the domain D of the Euclidean space $\mathcal{E}$ occupied by an atom—numbered 1 throughout this paragraph—of a pure substance and its first neighbours as a morphological characteristic of the material (the "unit cell", in crystallography), see Figure 2. According to the concepts defined in Section 2, the bond between atom 1 and one of its first neighbours, $j+1$, is fully characterized by the elementary conformation tensor $\boldsymbol{C}^{1,j+1} = \ln(\bar{r}^{1,j+1})\boldsymbol{N}^{1,j+1}$ where $\bar{r}^{1,j+1} = r^{1,j+1}/r_r$ and $\boldsymbol{N}^{1,j+1} = (\pm\boldsymbol{n}^{1,j+1}) \otimes (\pm\boldsymbol{n}^{1,j+1})$. The average conformation tensor $\widehat{\boldsymbol{C}}^1$ of atom 1 can then be simply defined as



$$\widehat{\boldsymbol{C}}^1 = \tfrac{1}{12}\textstyle\sum_{j=1}^{12} \boldsymbol{C}^{1,j+1} = \tfrac{1}{12}\sum_{j=1}^{12} \ln(\bar{r}^{1,j+1})\boldsymbol{N}^{1,j+1}$$

Figure 2 Example of a material domain (a "unit cell") D—an hexagonal close-packed pattern, here. The seven atomic nuclei—reduced to points in this study—belonging to the plane of the figure, including the central one numbered 1, are represented by black discs. An indication of the position of the six other atomic nuclei, which are out of the plane, is given by the grey discs. Each of them correspond to the projection, following $\boldsymbol{e}_3$ and in the plane $(1, \boldsymbol{e}_1, \boldsymbol{e}_2)$ of two atoms, one above the plane (numbered 8, for instance), the other one below the plane (numbered 11, for instance). Thus defined, the unit cell D is a cuboctahedron, i.e. a convex polyhedron with 14 faces and 12 inter-atomic bonds are to be taken into account, i.e. that of atom 1 with its 12 first neighbours. Each of these inter-atomic bonds is geometrically characterized by an elementary conformation tensor $\boldsymbol{C}^{1,j+1} = \ln(\bar{r}^{1,j+1})\boldsymbol{N}^{1,j+1}$, with $\bar{r}^{1,j+1} = r^{1,j+1}/r_r$ and $\boldsymbol{N}^{1,j+1} = (\pm\boldsymbol{n}^{1,j+1}) \otimes (\pm\boldsymbol{n}^{1,j+1})$, see also Equation (6). The average conformation tensor $\widehat{\boldsymbol{C}}^1$ is built from these elementary tensors as shown in the figure and Equation (12).

$$\widehat{\boldsymbol{C}}^1 = \frac{1}{N_l}\sum_{j=1}^{N_l} \boldsymbol{C}^{1,j+1} = \frac{1}{N_l}\sum_{j=1}^{N_l} \ln(\bar{r}^{1,j+1})\boldsymbol{N}^{1,j+1} \tag{12}$$

where N_l is the number of inter-atomic bonds of atom 1 (or, equivalently, the number of its first neighbours). In Figure 2, $N_l = 12$.

Like $\boldsymbol{C}$ in Equation (6), the tensor $\widehat{\boldsymbol{C}}^1$ is symmetric. Unlike $\boldsymbol{C}$, it has generally three different non-zero eigenvalues. Since it is defined as the sum of objective quantities, $\widehat{\boldsymbol{C}}^1$ is an objective quantity. Its trace is

$$\operatorname{Tr}\widehat{\boldsymbol{C}}^1 = \frac{1}{N_l}\sum_{j=1}^{N_l}(\boldsymbol{C}^{1,j+1}:\boldsymbol{G}) = \frac{1}{N_l}\sum_{j=1}^{N_l}\ln(\bar{r}^{1,j+1}) \tag{13}$$

where $\boldsymbol{G}$ is the metric tensor. Denoting by $\widehat{\bar{r}}$ the geometric mean of $\bar{r} = r/r_r$, the first invariant of $\widehat{\boldsymbol{C}}^1$ is then simply such that

$$\operatorname{Tr}\widehat{\boldsymbol{C}}^1 = \ln(\widehat{\bar{r}}^1) = \ln(\widehat{r}^1/r_r). \tag{14}$$

From this first result, a geometrical interpretation of the three eigenvalues $\hat{c}^{1k}$—which are real since $\widehat{\boldsymbol{C}}^1$ is symmetric—and the three eigenvectors $\hat{\boldsymbol{p}}^{1k}$—which are mutually orthogonal since $\widehat{\boldsymbol{C}}^1$ is symmetric—of the average conformation tensor can be deduced. The partition of $\widehat{\boldsymbol{C}}^1$ in spherical and deviatoric parts immediately gives

$$\widehat{\boldsymbol{C}}^1 : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) = \frac{1}{3}\operatorname{Tr}\widehat{\boldsymbol{C}}^1 + \mathbf{dev}(\widehat{\boldsymbol{C}}^1) : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) \tag{15}$$

or, equivalently, due to Equation (14):

$$\widehat{\boldsymbol{C}}^1 : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) = \frac{1}{3}\ln\left(\frac{\widehat{r}^1}{r_r}\right) + \mathbf{dev}(\widehat{\boldsymbol{C}}^1) : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) \tag{16}$$

from which we get, noting that $\widehat{\boldsymbol{C}}^1 : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) = \hat{c}^{1k}$ and $\mathbf{dev}(\widehat{\boldsymbol{C}}^1) : (\hat{\boldsymbol{p}}^{1k}\otimes\hat{\boldsymbol{p}}^{1k}) = \hat{c}_d^{1k}$:

$$r_r\exp(3\hat{c}^{1k}) = \widehat{r}^1\exp(3\hat{c}_d^{1k}) \tag{17}$$

where $\hat{c}_d^{1k}$ denotes the k–th eigenvalue of $\mathbf{dev}(\widehat{\boldsymbol{C}}^1)$. The geometrical interpretation of this result is given in the caption of Figure 3.

The energy of the N_l inter-atomic bonds of atom 1—in other words, the conformation energy of the discrete domain D—can be expressed as a function U of the N_l elementary conformation tensors $\boldsymbol{C}^{1,j+1}$. More precisely, so that the value of this function is an objective quantity, U can depend on:

- the Euclidean norm of the elementary conformation tensors—which are objective, see Section 2—, i.e. the distances $r^{1,j+1}$ between atom 1 and its N_l first neighbours—the single non-zero eigenvalue of the elementary conformation tensor $\boldsymbol{C}^{1,j+1}$ is indeed $\ln(\bar{r}^{1,j+1}) = \ln(r^{1,j+1}/r_r)$—, and
- the "crossed" invariants (Spencer 1971; Boehler 1987) of these elementary tensors—since these tensors are objective, their "crossed" invariants are also objective—, i.e. the angles between inter-atomic bonds. Indeed, the "crossed" invariant of the uniaxial tensors $\boldsymbol{C}^{1,p}$ and $\boldsymbol{C}^{1,q}$ simply reads

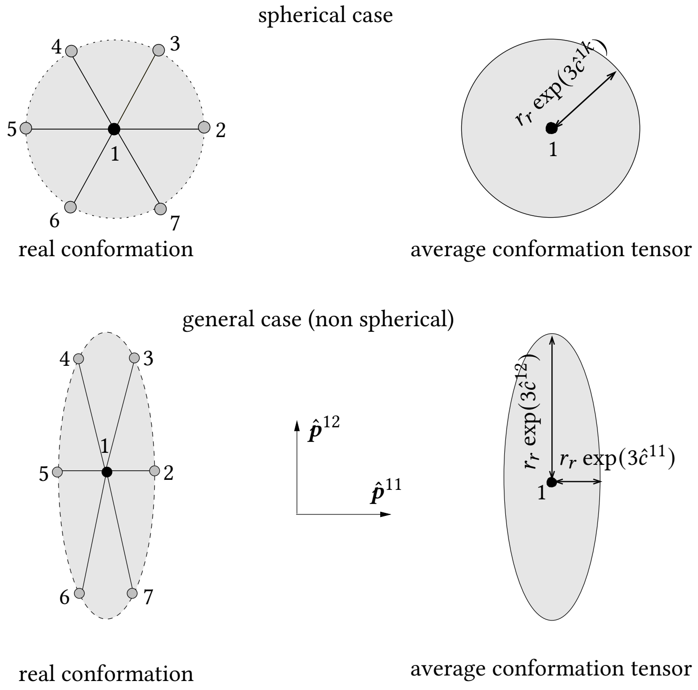
$$\boldsymbol{C}^{1,p} : \boldsymbol{C}^{1,p} = \ln(\bar{r}^{1,p})\ln(\bar{r}^{1,q})\;\boldsymbol{N}^{1,p} : \boldsymbol{N}^{1,q} = \ln(\bar{r}^{1,p})\ln(\bar{r}^{1,q})\cos^2(\omega^{p,q}) \tag{18}$$

where $\omega^{p,q}$ is the angle between inter-atomic bonds $1-p$ and $1-q$.
No particular expression of the multi-body potential U is given in this study. By contrast, it is postulated that there exists a state potential $\mathcal{U}$ of average free energy depending only on the average conformation tensor of the N_l inter-atomic bonds belonging to the unit cell D, $\widehat{\boldsymbol{C}}^1$, and such that

$$\mathcal{U}(\widehat{\boldsymbol{C}}^1) = \frac{1}{N_l}U(\boldsymbol{C}^{1,2},\boldsymbol{C}^{1,3},\dots,\boldsymbol{C}^{1,N_l+1}). \tag{19}$$

Following the procedure presented in Section 2, the average internal forces tensor acting on the inter-atomic bonds is then defined by

$$\widehat{\boldsymbol{F}}^1 = \frac{1}{\widehat{r}^1}\frac{\partial\mathcal{U}}{\partial\widehat{\boldsymbol{C}}^1}. \tag{20}$$


spherical case

general case (non spherical)

Figure 3 Interpretation of the eigenvalues and eigenvectors of the average conformation tensor. For the sake of simplicity, the figure is limited to the plane $(1, \boldsymbol{e}_1, \boldsymbol{e}_2)$, see Figure 2. The real (discrete) conformations of the inter-atomic bonds are on the left part of the figure, their representation according to the average conformation tensor, on the right part. The averaging process is inevitably accompanied by a loss of information which makes it impossible to know the position of the first neighbours (grey discs in the real conformation) of atom 1 (black disc). By contrast, it is possible to define the perimeter—the surface in $3D$—to which they belong on average. Thus, in the spherical case (upper part of the figure) where the three eigenvalues of the average conformation tensor are equal to $\hat{c}^{1k} = 1/3\ln(\hat{\bar{r}})$, the first neighbours of atom 1 belong in average to the circle of radius $\hat{r} = r_r\hat{\bar{r}} = r_r \exp(3\hat{c}^{1k})$. In the non spherical case (lower part of the figure), they belong to the ellipse with semi-axes $r_r \exp(3\hat{c}^{11})$ and $r_r \exp(3\hat{c}^{12})$ oriented along $\hat{\boldsymbol{p}}^{11}$ and $\hat{\boldsymbol{p}}^{12}$—in the $3D$ case, to the ellipsoid with semi-axes $r_r \exp(3\hat{c}^{11})$, $r_r \exp(3\hat{c}^{12})$ and $r_r \exp(3\hat{c}^{13})$, oriented along $\hat{\boldsymbol{p}}^{11}$, $\hat{\boldsymbol{p}}^{12}$ and $\hat{\boldsymbol{p}}^{13}$.

For the average free energy of the inter-atomic bonds to be an objective quantity, the state potential $\mathcal{U}$ must actually depend only on the three invariants of $\widehat{\boldsymbol{C}}^1$ or, equivalently, on its three eigenvalues. Since $\widehat{\boldsymbol{C}}^1$ and $\widehat{r}^1$ are objective quantities, $\widehat{\boldsymbol{F}}^1$ is an objective quantity. This symmetric tensor has generally three different, non-zero eigenvalues.

Three points can finally be emphasized about the average conformation tensor $\widehat{\boldsymbol{C}}^1$ and the average internal forces tensor $\widehat{\boldsymbol{F}}^1$, namely:

- The average conformation tensor can be defined if the considered pure substance has defects, punctual (*e. g.* vacancy defects) or linear (dislocations). In coherence with the assumption of elastic behavior retained in all these studies, it is only required that these defects are in constant number and, for dislocations at least, immobile.
- The directions of anisotropy $\pm\boldsymbol{n}^{1,j+1}$ (those represented by the line segments in Figure 2, for instance) could be simply taken into account by uniaxial tensors $\boldsymbol{N}^{1,j+1} = (\pm\boldsymbol{n}^{1,j+1}) \otimes (\pm\boldsymbol{n}^{1,j+1})$, with 1 as the single non-zero eigenvalue. The tensors $\boldsymbol{N}^{1,j+1}$ would then be new state variables on which the average free energy $\mathcal{U}$, see Equation (19), would depend, via "crossed" invariants (Boehler 1987), such that $\widehat{\boldsymbol{C}}^1 : \boldsymbol{N}^{1,j+1}$. The immediate consequence of such a choice would be that the tensor of average internal forces, $\widehat{\boldsymbol{F}}^1$, see Equation (20), and that of average conformation, $\widehat{\boldsymbol{C}}^1$, would not have the same eigenvectors. Although the mechanical behavior of crystalline structure, such as the one illustrated in Figure 2, is undoubtedly anisotropic, the directions of anisotropy $\boldsymbol{N}^{1,j+1}$ will be ignored in the following sections, in order to focus our attention on the main concept introduced in this study, namely the average conformation tensor of inter-atomic bonds.
- From the average internal forces tensor $\widehat{\boldsymbol{F}}^1$, the algebraic value of the average force acting on the

bond between atoms 1 and $j+1$, whose orientation is characterized by the tensor $\boldsymbol{N}^{1,j+1}$, is immediately deduced, which reads

$$\widehat{F}^{1,j+1} = \widehat{\boldsymbol{F}}^{1} : \boldsymbol{N}^{1,j+1}. \tag{21}$$

The net force resulting from all the forces exerted on atom 1 by its N_l neighbours being zero (static equilibrium), the latter are necessarily such that

$$\sum_{j=1}^{N_l} \widehat{F}^{1,j+1} \boldsymbol{N}^{1,j+1} = 0. \tag{22}$$

4 Average conformation tensor of inter-atomic bonds, average internal forces tensor and Cauchy stress tensor: continuum approach

The intrinsically atomistic nature of the matter has been taken into account in the discrete approach detailed in Section 3. However, this approach leads to a tensorial expression of the average internal forces from which it is not so easy to study the distribution of the forces in a given domain (a grain in a metallic material, for instance) and, in particular, how these forces are mutually balanced. It is therefore interesting to seek to associate to the real, discrete medium an equivalent continuous medium, fictitious, for which the equilibrium equations (balance of momentum) are well known, namely $\mathbf{div}_E\,(\boldsymbol{\sigma}) + \rho \boldsymbol{f}^m = 0$ where $\boldsymbol{f}^m$ is the density (per unit mass) of body forces ans where $\mathbf{div}_E$ denotes the Eulerian divergence.

In the present section and the following ones, any part of a pure substance in the solid state, whatever its volume, is therefore considered as a continuum medium. A continuous field of average conformation is supposed to exist in this domain. However, such a field is only physically relevant if its link with the real, discrete state of inter-atomic bonds is precisely defined. In a very first step, this requires to precise the scale at which the problem must be addressed. Since the average conformation tensor has been clearly defined for a nanoscopic domain (the unit cell), and only in this case, see Equation (12), the nanoscopic scale appears to be the right one. The fact that the matter, first of all its mass, has undoubtedly a discrete distribution at this scale does not seem to be a priori compatible with the idea of its description as a continuum. As we will see, this apparent incompatibility can be overcame, provided that the continuous field of average conformation is precisely defined, and then physically relevant.

A fictitious, continuum domain Δ is thus associated to the real, discrete unit cell D considered in Section 3. These two domains are said to be equivalent if and only if all the following conditions are verified:

- their volumes are equal: $\mathrm{vol}(D) = \mathrm{vol}(\Delta)$, see also Figure 4,
- the continuous field of average conformation acting in Δ, $\boldsymbol{\Gamma}(\boldsymbol{x})$, has “slow” spatial variations—in the sense that there exists a constant tensor $\boldsymbol{\Gamma}$ such that $\forall \boldsymbol{x} \in \Delta$, $\boldsymbol{\Gamma}(\boldsymbol{x}) \approx \boldsymbol{\Gamma}$—and is equal to the average conformation tensor defined in the discrete case—and therefore has the same physical meaning as it, cf. Section 3, in particular Figure 3: $\boldsymbol{\Gamma} = \widehat{\boldsymbol{C}}^1$,
- the energy of the discrete medium D—which reduces to the energy of the inter-atomic bonds in the present study—is equal to that of the continuum medium Δ. The calculation of this latter is based on the assumption that there exists a state potential of free energy density (per unit mass) Υ, depending only $\boldsymbol{\Gamma}$. Thus, from Equation (19), we have

$$U(\boldsymbol{C}^{1,2}, \boldsymbol{C}^{1,3}, \ldots, \boldsymbol{C}^{1,N_l+1}) = N_l \mathcal{U}(\widehat{\boldsymbol{C}}^1) \approx \int_\Delta \rho(\boldsymbol{x}) \Upsilon(\boldsymbol{\Gamma}) \mathrm{d}V. \tag{23}$$

As we will see later, the quasi-uniformity of the average conformation field acting in Δ implies that of the density ρ, see Section 5 and equation (44). We immediately infer that Equation (23) can be rewritten as

$$U(\boldsymbol{C}^{1,2}, \boldsymbol{C}^{1,3}, \ldots, \boldsymbol{C}^{1,N_l+1}) = N_l \mathcal{U}(\widehat{\boldsymbol{C}}^1) \approx \rho\, \mathrm{vol}(\Delta) \Upsilon(\boldsymbol{\Gamma}). \tag{24}$$

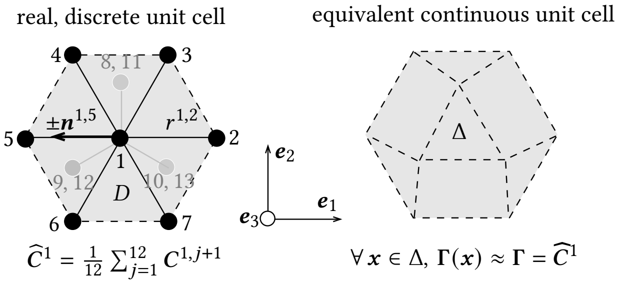


Figure 4 [Left] Example of a real, discrete domain D—the unit cell of an hexagonal close-packed pattern, as in Figure 2. [Right] Equivalent continuous unit cell Δ. The latter is said to be "equivalent" to the former insofar as: i) their volumes are equal: $\mathrm{vol}(D) = \mathrm{vol}(\Delta)$; ii) the continuous field of average conformation acting in Δ, $\boldsymbol{\Gamma}(\boldsymbol{x})$, is supposed to have "slow" spatial variations—consequently, $\boldsymbol{\Gamma}$ exists such that $\forall \boldsymbol{x} \in \Delta$, $\boldsymbol{\Gamma}(\boldsymbol{x}) \approx \boldsymbol{\Gamma}$; iii) the average conformation tensor associated to the real, discrete unit cell D, $\widehat{C}^1$, and the one characterizing approximately the continuous field of average conformation acting in Δ are equal: $\boldsymbol{\Gamma} = \widehat{C}^1$; iv) the mechanical energy of the inter-atomic bonds, which is the only energy considered in this study, is the same in the discrete case and in the continuous case. In other words, the free energy of D—$12\mathcal{U}(\widehat{C}^1)$, according to Equation (19)—and that of Δ are equal, as shown in Equation (24), where Υ denotes the state potential of free energy density (per unit mass), supposed to depend only on $\boldsymbol{\Gamma}$.

The average internal forces tensor acting on the inter-atomic bonds, actually being a density (per unit mass) of internal forces, is then given by, as in Section 3,

$$\boldsymbol{\Phi} = \frac{1}{\hat{r}} \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}} \tag{25}$$

where, according to Equation (14), $\hat{r} = r_r \exp(\mathrm{Tr}\,\boldsymbol{\Gamma})$. In strict logic, the internal forces define a continuous field in Δ, $\boldsymbol{\Phi}(\boldsymbol{x})$. However, like those of average conformation and density, this field is quasi-uniform and such that $\forall \boldsymbol{x} \in \Delta$, $\boldsymbol{\Phi}(\boldsymbol{x}) \approx \boldsymbol{\Phi}$.

If the state potential of average free energy density Υ depends only on the three invariants of $\boldsymbol{\Gamma}$, the quantity $\Upsilon(\boldsymbol{\Gamma})$ is objective. Since $\hat{r}$ is an objective quantity, $\boldsymbol{\Phi}$ is thus also an objective quantity. The average internal forces tensor as defined in Equation (25), however, is never taken into account in Continuum Mechanics, where the basic force-like quantity unanimously used is the Cauchy stress tensor, $\boldsymbol{\sigma}$. It is suggested here that the latter can be directly deduced from Equation (25), on the basis of a simple dimensional analysis. It reads as

$$\boldsymbol{\sigma} = \rho \hat{r} \boldsymbol{\Phi} = \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}}. \tag{26}$$

It has been underlined previously that Υ must actually depend on the three invariants of $\boldsymbol{\Gamma}$—and only on them if the anisotropy of the pure substance is not taken into account, which is the case in the present study, as stipulated in the last part of Section 3. If choosing the invariants $\mathrm{Tr}\,\boldsymbol{\Gamma}$, $\mathrm{Tr}(\boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma})$ and $\mathrm{Tr}(\boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma})$, the Cauchy stress tensor then reads

$$\boldsymbol{\sigma} = \rho \Big(\frac{\partial \Upsilon}{\partial \,\mathrm{Tr}\,\boldsymbol{\Gamma}} \boldsymbol{G} + 2 \frac{\partial \Upsilon}{\partial \,\mathrm{Tr}\,\boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma}} \boldsymbol{\Gamma} + 3 \frac{\partial \Upsilon}{\partial \,\mathrm{Tr}\,\boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma}} \boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma} \Big). \tag{27}$$

This equation shows that, in the case of isotropic elasticity, the average conformation tensor $\boldsymbol{\Gamma}$ and the Cauchy stress tensor $\boldsymbol{\sigma}$ have the same eigenvectors. Furthermore, as defined by Equation (26) or Equation (27), and since ρ, $\hat{r}$ and $\boldsymbol{\Phi}$ are objective quantities, $\boldsymbol{\sigma}$ is an objective quantity. However, above all, such a definition of the Cauchy stress tensor is a satisfactory answer to the central question asked in the present study, as shown in Equation (2): $\boldsymbol{S}$ denoting some strain tensor, $\boldsymbol{\Gamma} \neq \boldsymbol{S}$ exists—physically relevant and, especially, objective—and $\Upsilon(\boldsymbol{\Gamma})$ exists—is only supposed to exist, at the moment, with the general definition given by Equation (24)—such that $\boldsymbol{\sigma} = \rho \partial \Upsilon / \partial \boldsymbol{\Gamma}$. It must be recalled, however, that the stresses defined by Equation (26) are relative to a "frozen" state of a pure substance in the solid state, in other words, they do not take into account possible viscid effects.

There is a clear analogy between the previous definition of the Cauchy stress tensor and that, usual in Solid Mechanics, where the relation between $\boldsymbol{\sigma}$ and a strain tensor $\boldsymbol{S}$ is also obtained by differentiating a state potential of free energy density, see Equation (1). The two points of view differ in an essential way: when a strain tensor $\boldsymbol{S}$, whatever it is, is intrinsically linked to a reference configuration, see Section 1, the average conformation tensor $\boldsymbol{\Gamma}$ is independent of any reference configuration: its definition involves only a reference length $r_r \in \mathbb{R}^+$, which has been precisely defined in Section 2, i.e. for only two isolated atoms, interacting only with each other. In other words, the average conformation tensor is defined on the current configuration at any time t only (that of Δ on Figure 4 for example, that can be noted $\Delta_t \in \mathbb{R}^3$)—in the sense that it is not linked to any Lagrangian gradient—when a strain tensor is intrinsically linked to the transformation between a reference configuration (time t_r; $\Delta_r \in \mathbb{R}^3$ in the case of Figure 4) and the current configuration since it is built from the deformation gradient $\boldsymbol{T}$, see Section 1, which irreducibly links these two configurations, whatever the evolution between times t_r and t. It can be also noted that, more generally, no Lagrangian gradient of any physical quantity has been used in Sections 2 and 3 of this study, nor in the present section.

It should finally be noted that, if the transposition to the continuous case of the equilibrium equation of the discrete case, see Equation (22), is none other than the linear balance momentum equation, that is, in the quasi-static case and neglecting the mass forces, such as those due to gravity,

$$\mathbf{div}_E\,(\boldsymbol{\sigma}) = 0, \tag{28}$$

the relation between the Cauchy stress tensor $\boldsymbol{\sigma}$ (continuum case) and the inter-atomic forces discussed in Section 3, see Equation (21), is far from being obvious. This relation will not be studied in this paper, where the emphasis is clearly put on the geometrical notion of conformation. It should be studied in future studies, for instance based on (Parthasarathy et al. 2018) where the notions of static stress and vibration stress are defined at the atomic scale, on the basis of a refined description of atomic motions.

5 Thermodynamics and material derivative of the average conformation tensor of inter-atomic bonds

Like a strain tensor $\boldsymbol{S}$ in the classical, thermodynamic approach to the modeling of the mechanical behavior of materials in the solid state, the average conformation tensor of inter-atomic bonds defined in Section 4, $\boldsymbol{\Gamma}$, is now considered as a state variable. By contrast, and unlike the material derivative of $\boldsymbol{S}$, which is fully determined by the kinematics of the considered body, the material derivative of $\boldsymbol{\Gamma}$ is *a priori* unknown. The purpose of this section is to determine the latter, following a thermodynamic approach. As previously mentioned, however, it is here restricted to the elastic case. From a nanoscopic point of view, this means that, at any time of the evolution of the pure substance considered in the solid state:

- each atom has the same first neighbours. Defects such as dislocations can exist in the lattice, but in constant number and immobile (in other words, no plasticity),
- each atom is always bonded to its first neighbours by active inter-atomic bonds. These bonds can vary in length and direction but they cannot disappear or break (in other words, no damage).

Neglecting all the thermal effects (that is, in particular, $\dot{T} = 0$, where T is the absolute temperature and where $\dot{T}$ denotes its material derivative), the first law of the Thermodynamics reduces to (Coleman and Gurtin 1967; Garrigues 2007)

$$\rho \dot{e} = \boldsymbol{\sigma} : \boldsymbol{D} \tag{29}$$

where e is the state potential of the density (per unit mass) of average internal energy, depending only on $\boldsymbol{\Gamma}$ in the present case, and $\boldsymbol{D}$, the rate of deformation tensor, i.e. the symmetric part of the Eulerian velocity gradient.

The state potentials of the density of average internal energy e and of the average free energy Υ are related by $e = \Upsilon + sT$ where s is the state function of the density (per unit mass) of entropy. An alternative and local expression for the first law of the Thermodynamics, see Equation (29), is then immediately deduced, namely

$$\rho \dot{\Upsilon} + \rho T \dot{s} = \boldsymbol{\sigma} : \boldsymbol{D} \tag{30}$$

which can be rewritten, since Υ, like e, depends only on $\boldsymbol{\Gamma}$, as

$$\rho T\dot{s} = \boldsymbol{\sigma} : \boldsymbol{D} - \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}} : \dot{\boldsymbol{\Gamma}}. \tag{31}$$

The local expression of the second principle of the Thermodynamics—which expresses that the (per unit volume) dissipated power or intrinsic dissipation, ω, is non-negative—reads, in the isothermal case,

$$\omega = \rho T\dot{s} \geqslant 0, \quad \forall \boldsymbol{\Gamma}, \quad \forall \boldsymbol{D} \tag{32}$$

where the quantifiers indicate that this inequality must always be fulfilled, that is, whatever the mechanical state, $\boldsymbol{\Gamma}$, and whatever the evolution, $\boldsymbol{D}$. From Equation (31), Equation (32) can be immediately rewritten as

$$\omega = \boldsymbol{\sigma} : \boldsymbol{D} - \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}} : \dot{\boldsymbol{\Gamma}} \geqslant 0, \quad \forall \boldsymbol{\Gamma}, \quad \forall \boldsymbol{D} \tag{33}$$

or, equivalently, due to Equation (26),

$$\omega = \boldsymbol{\sigma} : (\boldsymbol{D} - \dot{\boldsymbol{\Gamma}}) \geqslant 0, \quad \forall \boldsymbol{\Gamma}, \quad \forall \boldsymbol{D}. \tag{34}$$

Therefore, the material derivative of the average conformation tensor turns out to be constrained by the Thermodynamics, that is to say that $\boldsymbol{\Gamma}$ is an internal state variable (Coleman and Owen 1974). By definition, the mechanical behavior of a material is referred to as elastic when the intrinsic dissipation ω is zero for all the states and evolutions. However, it should be kept in mind here that the material derivative of an objective, non scalar quantity, cannot be objective (Garrigues 2007). As is also the case for $\dot{\boldsymbol{\Gamma}}$, which is necessarily the sum of an objective part $\hat{\boldsymbol{\Gamma}}$—directly linked to the material derivative of its eigenvalues which, on the contrary, are objective—and a non objective part $\check{\boldsymbol{\Gamma}}$—due to the material derivative of its eigenvectors, which cannot be objective. With the hypothesis of elasticity, this latter remark makes it possible to write

$$\omega = \boldsymbol{\sigma} : (\boldsymbol{D} - \dot{\boldsymbol{\Gamma}}) = \boldsymbol{\sigma} : (\boldsymbol{D} - (\hat{\boldsymbol{\Gamma}} + \check{\boldsymbol{\Gamma}})) = 0, \quad \forall \boldsymbol{\Gamma}, \quad \forall \boldsymbol{D}. \tag{35}$$

A first condition for this equality to be ever verified is easy to get since the rate of deformation tensor, $\boldsymbol{D}$, is objective. It simply reads

$$\hat{\boldsymbol{\Gamma}} = \boldsymbol{D}. \tag{36}$$

It is not so immediate to give a mathematical expression for $\check{\boldsymbol{\Gamma}}$, knowing that its scalar product with $\boldsymbol{\sigma}$ must always be equal to zero, see Equation (35). The skew-symmetric part of the Eulerian velocity gradient, $\boldsymbol{W}$, is here helpful. It is such that, whatever the vector $\boldsymbol{a}$, the vector defined by $\boldsymbol{W} \cdot \boldsymbol{a}$ is orthogonal to $\boldsymbol{a}$. Applied to the eigenvectors of $\boldsymbol{\Gamma}$, $\boldsymbol{P}^k$—which are the same as those of the Cauchy stress tensor in the isotropic case, see Equation (27)—this inherent property of the skew-symmetric tensors ensures that the following symmetric tensor (γ^k denote the eigenvalues of $\boldsymbol{\Gamma}$):

$$\check{\boldsymbol{\Gamma}} = \sum_{k=1}^{3} \gamma^k ((\boldsymbol{W} \cdot \boldsymbol{P}^k) \otimes \boldsymbol{P}^k + \boldsymbol{P}^k \otimes (\boldsymbol{W} \cdot \boldsymbol{P}^k)) \tag{37}$$

is such that its scalar product with $\boldsymbol{\sigma}$ is always equal to zero, whatever the observer. Since $\boldsymbol{W}$ is a non objective quantity, $\check{\boldsymbol{\Gamma}}$ as defined by Equation (37) is a non objective quantity. From Equations (36) and (37), we immediately get that

$$\dot{\boldsymbol{\Gamma}} = \boldsymbol{D} + \sum_{k=1}^{3} \gamma^k ((\boldsymbol{W} \cdot \boldsymbol{P}^k) \otimes \boldsymbol{P}^k + \boldsymbol{P}^k \otimes (\boldsymbol{W} \cdot \boldsymbol{P}^k)) \tag{38}$$

is a condition for the intrinsic dissipation ω, see Equation (35), to be always zero, whatever the observer. It must however be noticed that this condition is sufficient but not necessary: by multiplying the second term on the right hand side of Equation (37) by any real number, another expression for $\check{\boldsymbol{\Gamma}}$ is obtained which is also such that its scalar product with $\boldsymbol{\sigma}$ is equal to zero. In any event, the expression for $\check{\boldsymbol{\Gamma}}$ must be such that its scalar product with $\boldsymbol{\sigma}$ is equal to zero. Accordingly, the power density (per unit volume) of internal forces, $\pi_{\mathrm{int}} = -\boldsymbol{\sigma} : \boldsymbol{D}$, can always be written as

$$\pi_{\mathrm{int}} = -\boldsymbol{\sigma} : \dot{\boldsymbol{\Gamma}}. \tag{39}$$

It may also be noted that, from the expression of the average conformation tensor in the orthonormal basis defined by its eigenvectors, namely

$$\boldsymbol{\Gamma} = \sum_{k=1}^{3} \gamma^k (\boldsymbol{P}^k \otimes \boldsymbol{P}^k) \tag{40}$$

which immediately gives the material derivative form

$$\dot{\boldsymbol{\Gamma}} = \sum_{k=1}^{3} \dot{\gamma}^k (\boldsymbol{P}^k \otimes \boldsymbol{P}^k) + \sum_{k=1}^{3} \gamma^k (\dot{\boldsymbol{P}}^k \otimes \boldsymbol{P}^k + \boldsymbol{P}^k \otimes \dot{\boldsymbol{P}}^k) \tag{41}$$

the objective part of $\dot{\boldsymbol{\Gamma}}$, according to Equation (36)—and due to the fact that the material derivatives of the eigenvalues γ^k are objective—, is such that

$$\hat{\boldsymbol{\Gamma}} = \boldsymbol{D} = \sum_{k=1}^{3} \dot{\gamma}^k (\boldsymbol{P}^k \otimes \boldsymbol{P}^k) \tag{42}$$

and the non objective part of $\dot{\boldsymbol{\Gamma}}$, according to Equation (37)—and due to the fact that the material derivatives of the eigenvectors $\boldsymbol{P}^k$ are non objective—is such that

$$\check{\boldsymbol{\Gamma}} = \sum_{k=1}^{3} \gamma^k ((\boldsymbol{W} \cdot \boldsymbol{P}^k) \otimes \boldsymbol{P}^k + \boldsymbol{P}^k \otimes (\boldsymbol{W} \cdot \boldsymbol{P}^k)) = \sum_{k=1}^{3} \gamma^k (\dot{\boldsymbol{P}}^k \otimes \boldsymbol{P}^k + \boldsymbol{P}^k \otimes \dot{\boldsymbol{P}}^k). \tag{43}$$

As defined by Equation (37) or Equation (43), $\check{\boldsymbol{\Gamma}}$ is a traceless tensor, i.e. $\operatorname{Tr} \dot{\boldsymbol{\Gamma}} = \operatorname{Tr} \boldsymbol{D}$. Furthermore, from the local expression of the law of conservation of mass, we also have $\operatorname{Tr} \boldsymbol{D} = -\dot{\rho}/\rho$. Consequently,

$$\operatorname{Tr} \dot{\boldsymbol{\Gamma}} = -\frac{\dot{\rho}}{\rho} \tag{44}$$

or, equivalently, due to Equation (14)—where $\boldsymbol{\Gamma}$ can be substituted to $\widehat{\boldsymbol{C}}^1$ since these two tensors are equal, see Section 4:

$$\frac{\dot{\widehat{r}}}{r_r} = -\frac{\dot{\rho}}{\rho}. \tag{45}$$

Denoting by ρ_0 (resp. by $\widehat{r}_0$) the density (resp. the average distance between the atomic nuclei) at some initial time, Equation (45) immediately gives

$$\frac{\widehat{r}}{\widehat{r}_0} = \frac{\rho_0}{\rho} \tag{46}$$

which means that, if $\rho \longrightarrow 0$, then $\widehat{r} \longrightarrow \infty$, and if $\rho \longrightarrow \infty$, then $\widehat{r} \longrightarrow 0$. Since the mass of an atom is essentially concentrated in its nucleus (see the very first part of Section 2), these two limit cases are formally satisfactory. It must be underlined, however, that they are physically irrelevant, at least in the present study: the first one, $\widehat{r} \longrightarrow \infty$, because the length of an inter-atomic bond, that is to say, the distance between two atomic nuclei, is always finite in the solid state; the second one, $\widehat{r} \longrightarrow 0$, because the fusion of atomic nuclei is obviously not an elastic phenomenon.

6 Example of an elasticity model based on the conformation tensor

As noted previously, the average conformation tensor, $\boldsymbol{\Gamma}$, is not a strain tensor, $\boldsymbol{S}$, because its definition does not depend upon any Lagrangian gradient. However, from an experimental point of view, it is not without interest to seek for a relationship between $\boldsymbol{\Gamma}$—at least some of its components—and $\boldsymbol{S}$, whatever this strain tensor is: at the microscopic scale, the tensor $\boldsymbol{S}$—at least some of its components—is indeed measurable when the tensor $\boldsymbol{\Gamma}$ is only accessible by measurements at the nanoscale. Such a relationship can be easily defined in the case of uniaxial tension, which is also interesting when the conformation variations (from an initial state of conformation) are "small" and reversible, in the sense that it suggests a certain mathematical expression of the state potential of specific free energy Υ introduced in Section 4. Consider the gauge section of a flat tensile specimen whose dimensions are defined in Figure 5 and whose constitutive material is a pure mono-atomic one. The pure metals are an example of such materials, which are however often, at the microscopic or larger scale, in the form of polycrystals, i.e. a set of crytallites or grains of varying sizes and orientations, and separated by grain boundaries. Obviously, the concept of conformation, and even more this of average conformation, introduced in the present study do not make sense physically on the interfaces that are the grain boundaries. So we must also assumed that the constitutive material of the specimen has no grain boundaries, which means that it is not only mono-atomic but also monocrystalline. In other words, the characteristic size of the specimen (e.g. L_0, see Figure 5) must be approximately this of the crystal of its constitutive material.

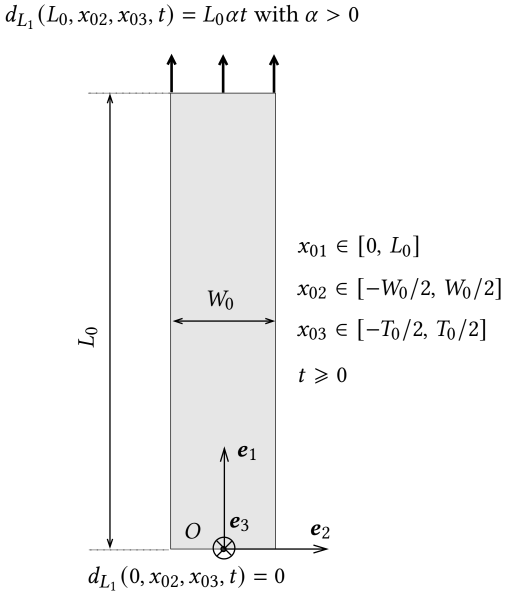


Figure 5 2D representation of the gauge section of a flat tensile specimen. The Lagrangian displacement field is denoted by $\boldsymbol{d}_L(\boldsymbol{x}_0, t)$, where $\boldsymbol{x}_0$ is the initial position vector—for the observer defined by point O and the orthonormal basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$—of some point of the gauge section, and where t denotes the time. The lateral edges of the gauge section are free from external stress while its upper and lower edges are such that only the components following $\boldsymbol{e}_2$ and $\boldsymbol{e}_3$ of the external stress vector are zero. Moreover, the constraint $d_{L_2}(x_{01}, 0, x_{03}, t) = 0$ is added to the kinematic boundary conditions to avoid any rigid body motion. All these boundary conditions and constraints are such that the Lagrangian gradient field of $\boldsymbol{d}_L$—and consequently, any strain field, whatever the considered strain tensor $\boldsymbol{S}$ is—is uniform in the entire gauge section. Eventually, it may be noted that, from the kinematic boundary condition on the upper edge of the gauge section, it is immediately deduced that αt is nothing else than the axial strain of the gauge section, usually denoted by ϵ_{11} in the case of infinitesimal strains.

Due to the kinematic boundary conditions, the Lagrangian description of the displacement field of the points of the gauge section, $\boldsymbol{d}_L$, is simple—for the observer defined by point O and the orthonormal basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, see Figure 5. It reads

$$\boldsymbol{d}_L(\boldsymbol{x}_0, t) = x_{01}\alpha t\boldsymbol{e}_1 + x_{02}g(t)\boldsymbol{e}_2 + x_{03}g(t)\boldsymbol{e}_3 \tag{47}$$

where $\alpha > 0$ and where the function $g(t)$, such that $g(t_0 = 0) = 0$ and $g'(t) < 0, \forall t$, does not have to be more specified here. From the Lagrangian gradient of $\boldsymbol{d}_L$, which defines a uniform field in the gauge section, the field of deformation gradient is immediately deduced, namely

$$\boldsymbol{T} = \mathbf{grad}_L\left(\boldsymbol{d}\right) + \boldsymbol{G} = (1 + \alpha t)(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1) + (1 + g(t))(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_3). \tag{48}$$

It may here be noted that any strain field, whatever the considered strain tensor $\boldsymbol{S}$, inherits the property of uniformity of $\boldsymbol{T}$, including the infinitesimal strain field:

$$\boldsymbol{\epsilon} = \alpha t(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1) + g(t)(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_3). \tag{49}$$

From Equation (47), the uniform field of the Eulerian velocity gradient $\boldsymbol{v}$ is also deduced:

$$\mathbf{grad}_E\left(\boldsymbol{v}\right) = \frac{\alpha}{1 + \alpha t}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1) + \frac{\dot{g}(t)}{1 + g(t)}(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_3). \tag{50}$$

Hence, since the tensor $\mathbf{grad}_E\left(\boldsymbol{v}\right)$ thus defined turns out to be symmetric:

$$\boldsymbol{D} = \mathbf{sym}(\mathbf{grad}_E\left(\boldsymbol{v}\right)) = \mathbf{grad}_E\left(\boldsymbol{v}\right), \quad \boldsymbol{W} = \mathbf{skw}(\mathbf{grad}_E\left(\boldsymbol{v}\right)) = 0. \tag{51}$$

The solution to Equation (38) governing the material derivative of $\boldsymbol{\Gamma}$ is then immediately obtained. It reads at any time (and at any point, since the field defined by $\boldsymbol{\Gamma}$ is uniform in the entire gauge section)

$$\begin{aligned}
&\Gamma_{11}(t) - \Gamma_{11}(0) = \ln(1 + \alpha t),\\
&\Gamma_{22}(t) - \Gamma_{22}(0) = \ln(1 + g(t)) = \Gamma_{33}(t) - \Gamma_{33}(0),\\
&\Gamma_{ij}(t) - \Gamma_{ij}(0) = 0 \text{ when } i \neq j.
\end{aligned} \tag{52}$$

There is no physical argument to claim that the initial state of average conformation $\boldsymbol{\Gamma}(0)$ vanishes. Quite the contrary, from Equation (17) and Figure 3, $\boldsymbol{\Gamma}(0) \neq \boldsymbol{0}$ describes a quite realistic physical condition, namely that the first neighbours of some atom initially belong to the ellipsoid with semi-axes $r_r \exp(3\gamma_0^1)$, $r_r \exp(3\gamma_0^2)$ and $r_r \exp(3\gamma_0^3)$, oriented along $\boldsymbol{P}_0^1$, $\boldsymbol{P}_0^2$ and $\boldsymbol{P}_0^3$ (here, γ_0^i denotes the i-th eigenvalue of $\boldsymbol{\Gamma}(0)$ and $\boldsymbol{P}_0^i$, its i-th eigenvector; it can also be recalled that r_r is a reference length). However, and in order to facilitate the presentation of the main results, it will be assumed here that $\boldsymbol{\Gamma}(0) = 0$—which is also a realistic condition, but very particular in the sense that the first neighbours of some atom initially belong to the sphere with a radius r_r. With this initial condition, $\Gamma_{11}(t)$ is nothing else than the true (natural) longitudinal strain, and $\Gamma_{22}(t) = \Gamma_{33}(t)$, the true transverse strain. But it is well known that the true strains, as long as they remain "small", are adequately approximated by the corresponding components of the infinitesimal strain tensor, see Equation (49). Thus, when $\alpha t \ll 1$ and $|g(t)| \ll 1$, Equation (52) simply becomes

$$\begin{aligned}
&\Gamma_{11}(t) \approx \epsilon_{11}(t) = \alpha t,\\
&\Gamma_{22}(t) = \Gamma_{33}(t) \approx \epsilon_{22}(t) = \epsilon_{33}(t) = g(t),\\
&\Gamma_{ij}(t) = \epsilon_{ij}(t) = 0 \text{ when } i \neq j.
\end{aligned} \tag{53}$$

In other words, in the case of uniaxial tension restricted to small strains, and for the observer defined by point O and the orthonormal basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, see Figure 5, $\boldsymbol{\Gamma} \approx \boldsymbol{\epsilon}$. In no way can this particular result be generalized, mainly because, as already mentioned, $\boldsymbol{\Gamma}$ is not a strain tensor. However, this same result suggests—but definitely not proves—that, in the case of small, elastic variations of conformation, that is to say when the eigenvalues of $\boldsymbol{\Gamma}$ are such that $|\gamma^k| \ll 1$, an expression of the average specific free energy of the inter-atomic bonds could be analogous to that underlying the very classical isotropic, linear elasticity model, namely

$$\Upsilon(\boldsymbol{\Gamma}) = \frac{1}{2\rho_0}(\lambda(\operatorname{Tr}\boldsymbol{\Gamma})^2 + 2\mu \operatorname{Tr}\boldsymbol{\Gamma}\cdot\boldsymbol{\Gamma}) \;\; \text{with} \;\; \mu > 0 \text{ and } \lambda > -\frac{2}{3}\mu \tag{54}$$

where ρ_0 is the initial density, and where λ and μ are analogous to the Lamé parameters. From Equation (54), and in agreement with the general expression of the Cauchy stress tensor previously defined, see Equation (26), we get

$$\boldsymbol{\sigma} = \frac{\rho}{\rho_0}(\lambda \operatorname{Tr} \boldsymbol{\Gamma} \boldsymbol{G} + 2\mu \boldsymbol{\Gamma}). \tag{55}$$

With the additional hypothesis that $\rho/\rho_0 \approx 1$, which is not inadmissible in the case of infinitesimal strains, Equation (55) is therefore equivalent to the famous Hooke's law, where the infinitesimal strain tensor is replaced by the average conformation tensor $\boldsymbol{\Gamma}$. But when Hooke's law is such that the initial stresses are zero—since, from the definition of the strains with respect to an initial state, the latter are zero at initial time –, the stresses defined by Equation (55) might well be non zero since the initial state of conformation has no reason to be zero—in Equation (53), it has been assumed that $\boldsymbol{\Gamma}(0) = \boldsymbol{0}$ only for the sake of brevity.

If one accepts, for "small" conformation variations, Equation (55) as isotropic, elasticity model, a generic structural problem based on the average conformation tensor can be formulated. In agreement with one of the main hypotheses adopted in this study, it relates only to structures whose constitutive material is a pure substance in the solid state. As always in the field of Mechanics, two equivalent formulations of the problem can be envisaged, a Lagrangian one and an Eulerian one. To highlight the fact that $\boldsymbol{\Gamma}$ is without any connection with the Lagrangian gradient of some vector field, the problem is here written in Eulerian description, for the material fields—such that $\boldsymbol{\Gamma}_E(\boldsymbol{x}_t, t)$, Eulerian field of the average conformation existing in the current configuration, Ω_t, of the considered structure—as well as for the differential operators—such that $\mathbf{div}_E\,(\boldsymbol{\sigma})$, Eulerian divergence of the stress field. The Eulerian field of the current position vector of the points of the considered structure is denoted by $\Xi_E(\boldsymbol{x}_t, t)$ (thus, trivially, $\Xi_E(\boldsymbol{x}_t, t) = \boldsymbol{x}_t$). The data of the problem are:

- the material parameters $\mu > 0$ and $\lambda > -(2/3)\mu$,
- the initial configuration for any observer of the considered structure, Ω_0,
- the initial fields of density $\rho_0(\boldsymbol{x}_0) = \rho_0$ of average conformation $\boldsymbol{\Gamma}_0(\boldsymbol{x}_0) = 0$, and of Cauchy stresses $\boldsymbol{\sigma}_0(\boldsymbol{x}_0) = \boldsymbol{0}$,
- the velocity field, $\boldsymbol{V}_t(\boldsymbol{x}_t)$, acting on the part $\partial\Omega_t^V$ of the current boundary $\partial\Omega_t$ of the structure, and the stress vector rate field, $\boldsymbol{f}_t(\boldsymbol{x}_t)$, acting on the part $\partial\Omega_t^f$ of $\partial\Omega_t$,
- the field of density of body forces, $\boldsymbol{f}^m(\boldsymbol{x}_t)$, acting in Ω_t, e.g. $\boldsymbol{f}^m = \boldsymbol{0}$ or $\boldsymbol{f}^m = \boldsymbol{g}$, gravitational acceleration.

The static equilibrium problem is then to find the current configuration, Ω_t, and the fields defined on the whole configuration $\Xi_E(\boldsymbol{x}_t, t)$, $\rho_E(\boldsymbol{x}_t, t)$, $\boldsymbol{\Gamma}_E(\boldsymbol{x}_t, t)$ and $\boldsymbol{\sigma}_E(\boldsymbol{x}_t, t)$ such that

$$\begin{aligned}
&\Omega_t = \{\Xi_E(\boldsymbol{x}_t, t) = \boldsymbol{x}_t\}\\
&\dot{\rho}_E = -\rho_E \operatorname{Tr} \mathbf{grad}_E\,(\dot{\Xi})\\
&\dot{\boldsymbol{\Gamma}}_E = \mathbf{sym}(\mathbf{grad}_E\,(\dot{\Xi})) + 2\sum_{k=1}^{3} \gamma_E^k \mathbf{sym}((\mathbf{skw}(\mathbf{grad}_E\,(\dot{\Xi})) \cdot \boldsymbol{P}_E^k) \otimes \boldsymbol{P}_E^k)\\
&\boldsymbol{\sigma}_E = \frac{\rho_E}{\rho_0}(\lambda \operatorname{Tr} \boldsymbol{\Gamma}_E \boldsymbol{G} + 2\mu \boldsymbol{\Gamma}_E)\\
&\mathbf{div}_E\,(\boldsymbol{\sigma}) + \rho_E \boldsymbol{f}^m = 0
\end{aligned} \tag{56}$$

satisfying the initial conditions ($t_0 = 0$)

$$\begin{aligned}
&\Omega_0 = \{\Xi_E(\boldsymbol{x}_0, 0) = \boldsymbol{x}_0\}\\
&\rho_E(\boldsymbol{x}_0, 0) = \rho_0(\boldsymbol{x}_0) \text{ in } \Omega_0\\
&\boldsymbol{\Gamma}_E(\boldsymbol{x}_0, 0) = \boldsymbol{\Gamma}_0(\boldsymbol{x}_0) \text{ in } \Omega_0\\
&\boldsymbol{\sigma}_E(\boldsymbol{x}_0, 0) = \boldsymbol{\sigma}_0(\boldsymbol{x}_0) \text{ in } \Omega_0,
\end{aligned} \tag{57}$$

along with the boundary conditions ($\boldsymbol{n}_E$ is the outward unit normal vector to $\partial\Omega_t^f$)

$$\dot{\Xi}_E(\boldsymbol{x}_t, t) = \boldsymbol{V}_t(\boldsymbol{x}_t) \text{ on } \partial\Omega_t^V, \quad \dot{\boldsymbol{\sigma}}_E(\boldsymbol{x}_t, t) \cdot \boldsymbol{n}_E(\boldsymbol{x}_t, t) = \boldsymbol{f}_t(\boldsymbol{x}_t) \text{ on } \partial\Omega_t^f \tag{58}$$

with $\partial\Omega_t^V \cap \partial\Omega_t^f = \emptyset$ and $\partial\Omega_t^V \cup \partial\Omega_t^f = \partial\Omega_t$.

In Equation (56), the number of equations is equal to the number of unknown fields—that is, 16 scalar fields, taking into account the symmetry of $\mathbf{\Gamma}$ and that of $\boldsymbol{\sigma}$—, which is a necessary condition for the static equilibrium problem to be well-posed. However, existence and uniqueness of solutions would require further study, which could be subjected to some constraints, in addition to that on the Lamé parameters, see Equation (54), and that on the boundary conditions, see Equation (58). In any case, it must be again emphasized that the structural problem here defined is different from the usual one, based on the infinitesimal strain tensor. Thus, it is inevitable that the solution of the latter, which involves only the symmetric part of the displacement Lagrangian gradient, is generally different from that of Equation (56), where both the symmetric and skew-symmetric parts of the velocity Eulerian gradient appear.

7 Conclusion

The three main results achieved in this study, in the case when a pure substance in the solid state is considered as a Continuum, are the following ones.

1. As a state variable, the average conformation tensor of inter-atomic bonds is an objective and relevant variable. Furthermore, and as opposed to a strain tensor, the average conformation tensor is independent of the transformation linking the current configuration to the reference (or initial) one.
2. Apart from the viscid effects, the Cauchy stress tensor can always be expressed as a function of the average conformation tensor, which is the first derivative of a state potential of the free energy density (per unit mass) of the inter-atomic bonds.
3. When the mechanical behavior of a pure substance can be considered as elastic, the objective part of the material derivative of the average conformation tensor is equal to the rate of deformation tensor.

However, for these results to be of a real importance in the field of Solid Mechanics, they must be expanded and/or enhanced from two points of view—in addition to the consideration of the second, the third, …, the umpteenth neighbours, which, however, is not a real problem, since an average conformation tensor, quite similar to that defined in this study, can be easily defined for each of these neighbours. The first is related to the class of materials to which these results can be actually applied. In the present paper, this class was restricted to pure substances in the solid state, in order to focus on the main idea of this study, as noted in Section 1. Nevertheless, the process followed in Sections 2 to 5 seems to be broad enough to be applied to materials which are not pure substances, that is to say, materials composed of at least two types of atoms. A precise theoretical study, however, aiming to prove that the notion of the average conformation tensor of inter-atomic bonds is relevant for this kind of materials in the solid state, still remains to be done.

Future studies should also investigate the problem of the irreversible mechanical behavior—in the sense of a non-zero intrinsic dissipation—of materials, which is always observed, whatever the material, when the supplied, mechanical energy becomes too high. More precisely, and considering that the thermodynamic results obtained in this study are valid in the only case of an elastic behavior, the following questions must be answered.

1. Which state variable(s) must be added to the average conformation tensor of inter-atomic bonds in a physically relevant model of the irreversible mechanical behavior (elastoplastic, for instance) of materials?
2. How is (are) the material derivative(s) of this (these) state variable(s), including that of the average conformation tensor of inter-atomic bonds, constrained by the Thermodynamics?

If precise and rigorous answers can be given to these questions, the average conformation tensor of inter-atomic bonds might become, as an alternative to a strain tensor, an interesting new state variable, in the essential sense that it is independent of the transformation linking the current configuration to the reference configuration, like the absolute temperature and the density.

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