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**The average conformation tensor of interatomic bonds as an alternative state variable to the strain tensor: definition and first application – the case of elasticity.**

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**Abstract**

This paper is a first attempt to formulate an elasticity model without any strain tensor. The new state variable introduced is the average conformation tensor of interatomic bonds. This variable is built from an elementary one – the conformation tensor of the interatomic bond linking two atoms of a pure substance –, firstly in the discrete case, then in the continuous case. In each of those cases, an average internal forces tensor is defined as the derivative of a free energy density, depending only on the new variable ; in the continuous case, the generic form of the Cauchy stress tensor is deduced. Assuming an elastic behavior, and following a thermodynamic approach, an expression for the material derivative of the new variable is also given. The average conformation tensor and a strain tensor are finally connected in the case of pure tension, from what an expression for the free energy density is inferred.

**Summary**

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 (e.g., [Adkins 1961]; [Fu and Ogden 2001]). However, one can ask whether an alternative state variable could not be considered. In the case of finite elastoplasticity (e.g., [Mandel 1971]; [Asaro 1983]; [Boyce et al. 1989]), the choice of a strain tensor as the basic, kinematic state variable is not totally without its problems, 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 interatomic bonds. The purpose, however, is restricted to a particular type of materials, namely the pure substances (copper or aluminium, for instance), and to the sole 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 bond can be characterized by a so called "conformation" tensor, and that the internal force acting on it can be fully described by a single scalar function, depending only on the conformation tensor: the state potential of free energy (or interaction potential). Using an averaging procedure, both these notions are then extended to a finite set of atoms, in other words to a "small" volume of a pure substance in the solid state considered as a discrete medium. They are also transposed to the Continuum case, where the atomic density (per unit mass) is first substituted to the finite set of atoms. An expression of the Cauchy stress tensor is deduced as the first derivative of a state potential of density (per unit mass) of average free energy of interatomic bonds, which is an explicit function of the average conformation tensor of in-

teratomic bonds. By applying a current procedure in Continuum Thermodynamics (e.g., [Coleman and Gurtin 1967]; [Garrigues 2007]), 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; Interatomic bonds; Conformation tensor; Continuum Mechanics; Cauchy stress tensor; Continuum Thermodynamics; Uniaxial tension; Elasticity model

### List of symbols

– **General symbols:**  $X \in \mathbb{R}$  denotes some scalar quantity,  $\mathbf{Y} \in \mathbb{R}^3$  some vectorial quantity and  $\mathbf{Z} \in \mathbb{R}^3 \times \mathbb{R}^3$  some tensorial quantity.

symbol	definition
$\mathbf{dev}(\mathbf{Z}) \in \mathbb{R}^3 \times \mathbb{R}^3$	deviatoric part of $\mathbf{Z}$ ; $\text{Tr}(\mathbf{dev}(\mathbf{Z})) = 0$
$\mathbf{G} \in \mathbb{R}^3 \times \mathbb{R}^3$	metric tensor (symmetric)
$\mathbf{sym}(\mathbf{Z}) = 1/2(\mathbf{Z} + \mathbf{Z}^T)$	symmetric part of $\mathbf{Z}$
$\mathbf{skw}(\mathbf{Z}) = 1/2(\mathbf{Z} - \mathbf{Z}^T)$	skew-symmetric part of $\mathbf{Z}$
$\text{Tr}(\mathbf{Z}) = \mathbf{Z}:\mathbf{G} \in \mathbb{R}$	first invariant of $\mathbf{Z}$ ; $\mathbf{Z} = \frac{1}{3} \text{Tr}(\mathbf{Z}) \mathbf{G} + \mathbf{dev}(\mathbf{Z})$
$\text{Tr}(\mathbf{Z}^2) = (\mathbf{Z}.\mathbf{Z}):\mathbf{G} \in \mathbb{R}_+$	second invariant of $\mathbf{Z}$ ; square of its Euclidean norm
$\text{Tr}(\mathbf{Z}^3) = (\mathbf{Z}.\mathbf{Z}.\mathbf{Z}):\mathbf{G} \in \mathbb{R}$	third invariant of $\mathbf{Z}$
$\dot{X}$ (resp. $\dot{\mathbf{Y}}$ or $\dot{\mathbf{Z}}$ )	material – Eulerian – derivative of $X$ (resp. of $\mathbf{Y}$ or $\mathbf{Z}$ )
$\mathbf{Z}^T \in \mathbb{R}^3 \times \mathbb{R}^3$	transpose of $\mathbf{Z}$

### – Symbols introduced in Section 2:

symbol	definition [Unit]
$\mathbf{C} \in \mathbb{R}^3 \times \mathbb{R}^3$	conformation tensor (symmetric, uniaxial) of an interatomic bond [ ]
$\mathbf{f} \in \mathbb{R}^3$	internal force vector of an interatomic bond [N]
$f \in \mathbb{R}$	algebraic value of $\mathbf{f}$ [N]
$\mathbf{F} \in \mathbb{R}^3 \times \mathbb{R}^3$	internal force tensor (symmetric, uniaxial) of an interatomic bond [N]
$\pm \mathbf{n} \in \mathbb{R}^3$	unit vector characterizing the direction of an interatomic bond [ ]
$\mathbf{N} = (\pm \mathbf{n}) \otimes (\pm \mathbf{n})$	direction tensor (symmetric, uniaxial) of an interatomic bond [ ]
$r \in \mathbb{R}_+^*$	distance between two atomic nuclei, or length of the bond linking two atoms [m]
$r_r \in \mathbb{R}_+^*$	reference length, e.g., this of an interatomic bond when no force is applied [m]
$\bar{r} = r/r_r \in \mathbb{R}_+^*$	normalized length of an interatomic bond [ ]

symbol	definition [Unit]
$u$	state potential of free energy of an interatomic bond or interaction potential [ $J$ ]
$u(\mathbf{C}) \in \mathbb{R}$	free energy of a $\mathbf{C}$ -conformed interatomic bond [ $J$ ]

– Symbols introduced in Section 3:

symbol	definition [Unit]
$\mathbf{C}^{i,j} = \ln(\bar{\mathbf{r}}^{i,j})\mathbf{N}^{i,j} \in \mathbb{R}^3 \times \mathbb{R}^3$	conformation tensor (symmetric, uniaxial) of the bond between atom $i$ and atom $j$ in $d$ [ ]
$\langle \mathbf{C}^i \rangle \in \mathbb{R}^3 \times \mathbb{R}^3$	average conformation tensor (symmetric) of the interatomic bonds formed by atom $i$ of $d$ [ ]
$\hat{\mathbf{C}} \in \mathbb{R}^3 \times \mathbb{R}^3$	average conformation tensor (symmetric) of the interatomic bonds formed by the atoms in $d$ [ ]
$\hat{c}^k \in \mathbb{R}$	$k$ –th eigenvalue of $\hat{\mathbf{C}}$ [ ]
$D \subset \mathcal{E}$	domain occupied by a pure substance in the solid state considered as a discrete medium [ ]
$\partial D$	boundary of $D$ [ ]
$d \subset D$	subdomain of $D$ , such that $\partial d \cap \partial D = \emptyset$ [ ]
$\hat{\mathbf{F}} \in \mathbb{R}^3 \times \mathbb{R}^3$	average internal forces tensor (symmetric) of the interatomic bonds in $d$ [ $N$ ]
$n_i \in \mathbb{N}^*$	number of interatomic bonds formed by atom $i$ in $d$ [ ]
$N_a \in \mathbb{N}^*$	number of atoms in $d$ [ ]
$N_l \in \mathbb{N}^*$	number of interatomic bonds in $d$ [ ]
$\mathbf{N}^{i,j} \in \mathbb{R}^3 \times \mathbb{R}^3$	direction tensor (symmetric, uniaxial) of the bond between atom $i$ and atom $j$ in $d$ [ ]
$\hat{\mathbf{p}}^k \in \mathbb{R}^3$	$k$ –th eigenvector of $\hat{\mathbf{C}}$ [ ]
$r^{i,j} \in \mathbb{R}_+^*$	length of the bond between atom $i$ and atom $j$ in $d$ [ $m$ ]
$\bar{r}^{i,j} = r^{i,j}/r_r \in \mathbb{R}_+^*$	normalized length of the bond between atom $i$ and atom $j$ in $d$ [ ]
$\hat{\bar{r}} \in \mathbb{R}_+^*$	average, normalized length of the interatomic bonds in $d$ [ ]
$U(\mathbf{C}^{i,j}, \dots, \mathbf{C}^{i,j} : \mathbf{C}^{i,j+1}, \dots)$	free energy of the interatomic bonds acting in $d$ [ $J$ ]
$\mathcal{U}(\hat{\mathbf{C}}) \in \mathbb{R}$	average free energy of the interatomic bonds in $d$ [ $J$ ]

– Symbols introduced in Section 4:

symbol	definition [Unit]
$\mathbf{\Gamma} \in \mathbb{R}^3 \times \mathbb{R}^3$	average conformation tensor (symmetric) of the interatomic bonds at point $P$ [ ]
$\gamma^k \in \mathbb{R}$	$k$ -th eigenvalue of $\mathbf{\Gamma}$ [ ]
$\mathcal{D} \subset \mathcal{E}$	domain occupied by a pure substance in the solid state considered as a continuum [ ]
$\delta_l(\bar{r}, \mathbf{N}) \in \mathbb{R}_+$	density (per unit mass) of $(\bar{r}, \mathbf{N})$ - conformed interatomic bonds at point $P$ [ $kg^{-1}$ ]
$\Delta_a = m_a^{-1} \in \mathbb{R}_+^*$	density (per unit mass) of atoms at point $P$ [ $kg^{-1}$ ]
$\Delta_l \in \mathbb{R}_+^*$	density (per unit mass) of interatomic bonds at point $P$ [ $kg^{-1}$ ]
$\mathbb{E}_c = \mathbb{R}_+^* \times \mathbb{E}_N$	conformation space [ ]
$\mathbb{E}_N \subset \mathbb{R}^3 \times \mathbb{R}^3$	direction space [ ]
$\mathbf{H}(\bar{r}) \in \mathbb{R}^3 \times \mathbb{R}^3$	tensor (symmetric) of density (per unit mass) of $\bar{r}$ - long interatomic bonds at point $P$ [ $kg^{-1}$ ]
$m_a \in \mathbb{R}_+^*$	atomic mass of the considered pure substance [ $kg$ ]
$n_l(\bar{r}, \mathbf{N}) \in \mathbb{R}_+$	number of $(\bar{r}, \mathbf{N})$ - conformed interatomic bonds at point $P$ [ ]
$P \in \mathcal{D}$	some point in $\mathcal{D}$ [ ]
$\mathbf{P}^k \in \mathbb{R}^3$	$k$ -th eigenvector of $\mathbf{\Gamma}$ [ ]
$\rho \in \mathbb{R}_+^*$	density at point $P$ [ $kg.m^{-3}$ ]
$\boldsymbol{\sigma} \in \mathbb{R}^3 \times \mathbb{R}^3$	Cauchy stress tensor (symmetric) at point $P$ [ $Pa$ ]
$\Upsilon$	state potential of density (per unit mass) of average free energy of interatomic bonds at point $P$ [ $J.kg^{-1}$ ]
$\Upsilon(\mathbf{\Gamma}) \in \mathbb{R}$	density (per unit mass) of average free energy of interatomic bonds at point $P$ [ $J.kg^{-1}$ ]
$V \in \mathbb{R}_+^*$	volume of $\mathcal{D}$ [ $m^3$ ]
$V_N \in \mathbb{R}_+^*$	volume of the direction space [ ]
$\boldsymbol{\Phi} \in \mathbb{R}^3 \times \mathbb{R}^3$	average internal forces (per unit mass) tensor (symmetric) at point $P$ [ $N.kg^{-1}$ ]
$\mathbf{X} \in \mathbb{R}^3 \times \mathbb{R}^3$	some strain tensor at point $P$ [ ]

– Symbols introduced in Section 5:

symbol	definition [Unit]
$\mathbf{D} \in \mathbb{R}^3 \times \mathbb{R}^3$	symmetric part of the velocity (Eulerian) gradient or rate of deformation tensor at point $P$ [ $s^{-1}$ ]
$e$	state potential of density (per unit mass) of average internal energy of interatomic bonds at $P$ [ $J.kg^{-1}$ ]
$s$	state function of density (per unit mass) of entropy at point $P$ [ $J.kg^{-1}.K^{-1}$ ]
$T \in \mathbb{R}_+^*$	absolute temperature at point $P$ [ $K$ ]
$\omega \in \mathbb{R}_+^*$	density (per unit volume) of intrinsic dissipation at point $P$ [ $W.m^{-3}$ ]
$\mathbf{W} \in \mathbb{R}^3 \times \mathbb{R}^3$	skew-symmetric part of the velocity (Eulerian) gradient at point $P$ [ $s^{-1}$ ]

– Symbols introduced in Section 6:

symbol	definition [Unit]
$\mathbf{d}_L(\mathbf{x}_0, t) \in \mathbb{R}^3$	Lagrangian displacement field [ $m$ ]
$\boldsymbol{\epsilon} \in \mathbb{R}^3 \times \mathbb{R}^3$	infinitesimal strain tensor [ ]
$t \in \mathbb{R}$	time [ $s$ ]
$\mathbf{T} \in \mathbb{R}^3 \times \mathbb{R}^3$	deformation gradient (Lagrangian) field [ ]
$\mathbf{v}_E(\mathbf{x}_t, t) \in \mathbb{R}^3$	Eulerian velocity field [ $m.s^{-1}$ ]
$\mathbf{x}_0 \in \mathbb{R}^3$	initial position vector [ $m$ ]
$\mathbf{x}_t \in \mathbb{R}^3$	current position vector [ $m$ ]
$\boldsymbol{\Xi}_E(\mathbf{x}_t, t) \in \mathbb{R}^3$	Eulerian position field [ $m$ ]

## 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  $\mathbf{X}$  and, if necessary, to so called internal variables (e.g., [Coleman and Gurtin 1967]), 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  $\psi$ , namely:

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \mathbf{X}} \quad (1)$$

where  $\rho$  is the density of the material. Thus, like the eventual internal variables – and, in Thermomechanics, the temperature –, a strain tensor  $\mathbf{X}$  is one of the variables on which  $\psi$  depends, in other words, it is a state variable. Since the pioneer work of, among others, [Eringen 1967], this way of building a mechanical model has been widely and successfully used. Most of the proven mechanical models are built in such a way. They are sometimes called – at least in the isotropic, elastic case, for which  $\mathbf{X}$  is the only state variable to be taken into account – hyper-elastic models to underline that the  $\boldsymbol{\sigma}$  –  $\mathbf{X}$  relation derives from a state potential (e.g. [Adkins 1961]; [Fu and Ogden 2001]). The important point that must be emphasized here 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 innumerable numerical simulations based on mechanical models obeying Eq.1 most often lead to physically relevant results. But neither the experiments, nor the numerical simulations definitely prove that a strain tensor  $\mathbf{X}$  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  $\mathbf{X}$  could be used to express the stress tensor  $\boldsymbol{\sigma}$  is therefore not meaningless.

The same question is both relevant and interesting when mechanical models more advanced than elasticity models are considered, where, in addition to  $\mathbf{X}$ , other state variables (the internal variables) have to be taken into account. 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  $\mathbf{T}$  must be multiplicatively decomposed into an elastic part,  $\mathbf{T}^e$ , and a plastic part,  $\mathbf{T}^p$ . In the vast majority of cases, the following decomposition is selected :  $\mathbf{T} = \mathbf{T}^e \cdot \mathbf{T}^p$  (e.g., [Mandel 1971]; [Asaro 1983]; [Boyce et al. 1989]). But it has to be said that this choice is never clearly justified, either kinematically or physically. Moreover, this way of decomposing  $\mathbf{T}$  presupposes the existence of a so-called intermediate configuration of the considered solid, which acts as a reference configuration for the calculation of  $\mathbf{T}^e$ . Nevertheless, when the initial (reference) and current configurations are pure geometrical, kinematical concepts, the intermediate configuration can be defined only on the basis of a condition on the internal forces, namely that the stress field is zero, 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, whatever 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,  $\mathbf{X}^p$ , and an elastic deformation tensor,  $\mathbf{X}^e$ , are proposed. As for the elastoplasticity models based on an additive decomposition of the rate of deformation tensor,  $\mathbf{D}$ , in an elastic part,  $\mathbf{D}^e$ , and a plastic part,  $\mathbf{D}^p$  (e.g., [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  $\mathbf{X}^e$  and  $\mathbf{X}^p$ . At worst, they sow doubt on their physical relevancy. At the very least, this calls for considering that the choice of the deformation (Lagrangian) gradient tensor  $\mathbf{T}$  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  $\mathbf{\Gamma}$  in the continuous case –, as an alternative to a strain tensor  $\mathbf{X}$  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  $\mathbf{\sigma}$ , the main question asked in this paper is the following one:

does  $\mathbf{\Gamma} \neq \mathbf{X}$  exist and does  $\Upsilon(\mathbf{\Gamma}, \dots)$  exist such that

$$\mathbf{\sigma} = \rho \frac{\partial \Upsilon}{\partial \mathbf{\Gamma}} ? \quad (2)$$

where  $\Upsilon$  denotes the state potential of Helmholtz free energy density (per unit mass), and where the state variable  $\mathbf{\Gamma}$ , if it exists, must be physically relevant and, especially, objective (e.g., [Eringen 1967]; [Murdoch 2003]; [Liu 2004]). For the sake of enhancement of the main, new ideas, the question asked in Eq. (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. Moreover – and 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 –, the present study is limited to the elastic case.

The paper is organized as follows: two atoms of a pure substance in the solid state, that is to say, linked by an interatomic bond, are considered in Section 2, in order to precisely define the basic kinematical and force-like quantities, namely, the conformation tensor of the interatomic bond and the associated, internal force tensor. The discrete modeling of a finite set of atoms of a pure substance in the solid state, where each atom has interatomic bonds with some of his neighbors, is discussed in Section 3. Both the ideas exposed in Section 2 are generalized by defining the average conformation tensor of interatomic bonds and the associated, average internal forces tensor. Section 4 is devoted to the Continuum description of a pure substance in the solid state. The finite, discrete set of atoms is first replaced by the density (per unit mass) of atoms, which is a continuous, uniform field. In full agreement with the assumption of a continuous distribution of mass, two continuous quantities are defined: the average conformation tensor of interatomic bonds and the associated, average internal forces tensor (per unit mass). Directly linked to the latter, a definition is also 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. Finally, Section 6 examines the uniaxial tension test, 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 Conformation tensor of an interatomic bond and internal force tensor: definitions

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 "interatomic bond" (*e.g.*, a metallic bond). The characteristic size of these atoms is given by the Bohr radius, which is approximately  $5 \times 10^{-2}nm$ , when the radius of an atomic nucleus is approximately  $5 \times 10^{-7}nm$ : 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  $r$  –

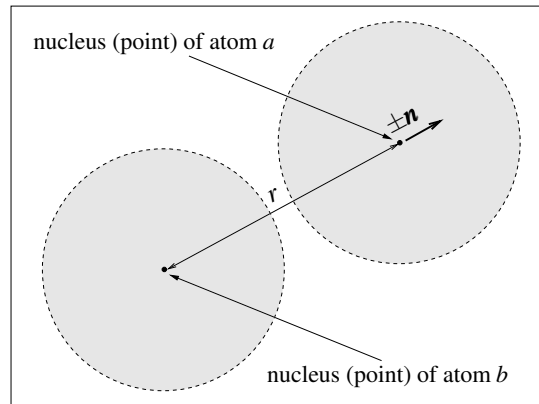


Figure 1: 2D, schematic representation of two atoms,  $a$  and  $b$ , of a pure substance in the solid state and of the interatomic bond linking  $a$  and  $b$ . The mass of each atom is mainly concentrated in its nucleus, which is considered as a point. The distance between the nuclei is denoted by  $r$ , the unit vector of the direction defined by the nuclei, by  $\pm \mathbf{n}$ . The dashed circles provide a simplistic image of the electron clouds.

which has the same value for all the observers in classical physics – and the unit vector of the direction defined by the nuclei, by  $\pm \mathbf{n}$ , see Fig. 1. Both these quantities are objective,

and their product,  $\pm r\mathbf{n}$ , is nothing other 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, which will be denoted by  $r_r$  in the remainder of the study. Then, the normalized length of the interatomic bond – or, equivalently, the normalized distance between the two nuclei – is defined by:

$$\bar{r} = \frac{r}{r_r} \quad (3)$$

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

$$\mathbf{N} = \mathbf{n} \otimes \mathbf{n} = (-\mathbf{n}) \otimes (-\mathbf{n}) \quad (4)$$

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

$$\text{Tr}(\mathbf{N}) = \text{Tr}(\mathbf{N}^2) = \text{Tr}(\mathbf{N}^3) = 1$$

In other words,  $\mathbf{N}$  is a uniaxial tensor with 1 as sole non-zero eigenvalue. The conformation tensor of the interatomic bond is then defined by:

$$\mathbf{C} = \ln(\bar{r})\mathbf{N} \quad (5)$$

The only non-zero eigenvalue of the symmetric tensor  $\mathbf{C}$  defined by Eq. (5) is  $\ln(\bar{r})$ . In other words,  $\mathbf{C}$  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 interatomic 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". 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 Eq. (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:

$$f = p'(r) = \frac{1}{r_r} q'(\bar{r}) \quad (6)$$

since  $\bar{r} = r/r_r$ , see Eq. (3). In Eq. (6),  $p'$  (resp.  $q'$ ) denotes the first derivative of  $p$  (resp. of  $q$ ). Hereafter in this study, it will be conventionally assumed 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,  $\pm\mathbf{n}$ . Hence, the internal force vector is given by  $\mathbf{f} = \pm f\mathbf{n}$ . Like the vector of the relative position of the two nuclei,  $\pm r\mathbf{n}$ ,  $\mathbf{f}$  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  $u(\mathbf{C})$ . For the value of this function for a given conformation tensor  $\mathbf{C}$  to be an objective quantity, the state potential  $u$  must depend only on the invariants of  $\mathbf{C}$ , which are linked, as previously

mentioned. The square of the Euclidean norm of the conformation tensor,  $\mathbf{C}:\mathbf{C} = \ln^2(\bar{r})$ , is then considered as the only variable on which  $u$  depends. Obviously, the state of free energy of the interatomic bond is the same whether the state potential of free energy is expressed as a function of  $r$  or  $\bar{r}$  or  $\mathbf{C}$ . Thus, the following relation is necessarily verified:

$$u(\mathbf{C}:\mathbf{C}) = q(\bar{r}) = p(r(\bar{r}))$$

Given that:

$$2 \frac{\ln(\bar{r})}{\bar{r}} u' = r_r p' = q' = r_r f \quad (7)$$

where  $u'$  denotes the first derivative of  $u$ , and given also that, in agreement with Eq. (5):

$$\frac{\partial u}{\partial \mathbf{C}} = u' \frac{\partial (\mathbf{C}:\mathbf{C})}{\partial \mathbf{C}} = 2u' \mathbf{C} = 2 \ln(\bar{r}) u' \mathbf{N}$$

the following internal force tensor can then be defined, according to Eq. (7):

$$\mathbf{F} = \frac{1}{r} \frac{\partial u}{\partial \mathbf{C}} = f \mathbf{N} \quad (8)$$

As a matter of fact, the symmetric tensor  $\mathbf{F}$  has a single non-zero eigenvalue,  $p'(r)$ , which is the algebraic value  $f$  of the internal force usually considered, see Eq. (6). Note also that all the quantities appearing on the right hand side of Eq. (8) are objective. As a consequence,  $\mathbf{F}$  is an objective quantity.

### 3 Average conformation tensor of interatomic bonds and average internal forces tensor: discrete case

Let  $D$  be the domain of the Euclidean space  $\mathcal{E}$  occupied by a pure substance in the solid state, considered to be a discrete medium. The boundary of  $D$  is denoted by  $\partial D$ . Let  $d$  be a subdomain of  $D$ , containing  $N_a \gg 1$  atoms, see Fig. 2. For the sake of simplification, it will be subsequently assumed that  $d$  is strictly inside  $D$ , in the sense that  $\partial d \cap \partial D = \emptyset$ . Any  $i$  atom belonging to  $d$  has one interatomic bond with some of its neighbors, the first ones but also, at least in the case of metallic materials, the second if not the third ones. However, the interactions between atom  $i$  and its first neighbors are dominant. In any case, these dominant interactions are the only which will be considered thereafter. They will be referred to as "active". Their number is denoted by  $n_i$ . According to the concepts defined in Section 2, the bond between atom  $i$  and atom  $j$  is fully characterized by the conformation tensor  $\mathbf{C}^{i,j} = \ln(\bar{r}^{i,j}) \mathbf{N}^{i,j}$ , where  $\bar{r}^{i,j} = r^{i,j}/r_r$  and  $\mathbf{N}^{i,j} = (\pm \mathbf{n}^{i,j}) \otimes (\pm \mathbf{n}^{i,j})$ . Assuming that two atoms which are not first neighbors have a zero conformation tensor ("non active" bond), the average conformation tensor of atom  $i$ ,  $\langle \mathbf{C}^i \rangle$ , can then be simply defined in the following way:

$$\langle \mathbf{C}^i \rangle = \frac{1}{n_i} \sum_{j=1}^{N_a} \mathbf{C}^{i,j} = \frac{1}{n_i} \sum_{j=1}^{N_a} \ln(\bar{r}^{i,j}) \mathbf{N}^{i,j}$$

Like  $\mathbf{C}$  in Eq. (5), the tensor  $\langle \mathbf{C}^i \rangle$  is symmetric. Unlike  $\mathbf{C}$ , it has generally three different non-zero eigenvalues. Since it is defined as the sum of objective quantities,  $\langle \mathbf{C}^i \rangle$  is an objective quantity.

In the same way as for atom  $i$ , an average conformation tensor of interatomic bonds can be obviously associated with all the other atoms belonging to  $d$ . As a consequence, an average conformation tensor of interatomic bonds of the  $N_a$  atoms belonging to  $d$  can be defined, which reads:

$$\hat{\mathbf{C}} = \frac{1}{2N_l} \sum_{i=1}^{N_a} \sum_{j_i=1}^{N_a} \mathbf{C}^{i,j_i} = \frac{1}{2N_l} \sum_{i=1}^{N_a} n_i \langle \mathbf{C}^i \rangle \quad \text{with } N_l = \frac{1}{2} \sum_{i=1}^{N_a} n_i \quad (9)$$

where  $N_l$  is interpreted as the total number of interatomic bonds acting in  $d$ . In Eq. (9), the multiplicative factor  $1/2$  is due to the fact that each interatomic bond appears twice since  $\mathbf{C}^{i,j_i} = \mathbf{C}^{j_i,i}$ , and, by convention,  $\mathbf{C}^{i,i} = 0$ . Like  $\langle \mathbf{C}^i \rangle$ , the tensor  $\hat{\mathbf{C}}$  is symmetric. It generally has three different non-zero eigenvalues. Since it is defined as the sum of objective quantities, it is an objective quantity. The trace of  $\hat{\mathbf{C}}$  is given by ( $\mathbf{G}$  is the metric

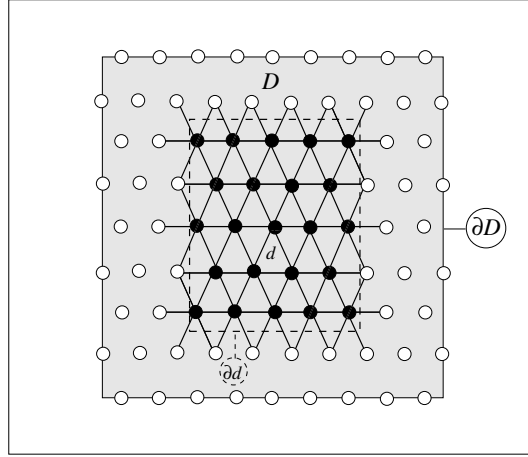


Figure 2: 2D illustration of a pure substance in the solid state, considered to be a discrete medium. The domain  $D$  (85 atoms, whose nuclei, represented here by white and black discs, are highly magnified) to which the pure substance belongs is the grey square. An example of the domain  $d \subset D$  on which the average conformation tensor can be calculated, see Eq. (9), is the rectangle delimited by the dashed line. All the atoms belonging to  $d$  (black discs ; total number  $N_a = 23$ ) have 6 first neighbors or, equivalently, 6 active interatomic bonds (here represented by line segments ; total number  $N_l = 69$ ). Note that this is not the case for the atoms belonging to the boundary of  $D$  (only 3 or 4 first neighbors), which would require further attention.

tensor):

$$\text{Tr}(\hat{\mathbf{C}}) = \frac{1}{2N_l} \sum_{i=1}^{N_a} \sum_{j_i=1}^{N_a} (\mathbf{C}^{i,j_i} : \mathbf{G}) = \frac{1}{2N_l} \sum_{i=1}^{N_a} \sum_{j_i=1}^{N_a} \ln(\bar{r}^{i,j_i})$$

Denoting by  $\hat{r}$  the geometric mean of  $\bar{r} = r/r_r$ , the first invariant of  $\hat{\mathbf{C}}$  is then simply such that:

$$\text{Tr}(\hat{\mathbf{C}}) = \ln(\hat{r}) = \ln\left(\frac{\hat{r}}{r_r}\right) \quad (10)$$

From this first result, a geometrical interpretation of the three eigenvalues  $\hat{c}^k$  – which are real since  $\hat{\mathbf{C}}$  is symmetric – and the three eigenvectors  $\hat{\mathbf{p}}^k$  – which are mutually orthogonal since  $\hat{\mathbf{C}}$  is symmetric – of the average conformation tensor can be deduced. The partition

of  $\hat{\mathbf{C}}$  in spherical and deviatoric parts immediately gives:

$$\hat{\mathbf{C}} : (\hat{\mathbf{p}}^k \otimes \hat{\mathbf{p}}^k) = \frac{1}{3} \text{Tr}(\hat{\mathbf{C}}) + \text{dev}(\hat{\mathbf{C}}) : (\hat{\mathbf{p}}^k \otimes \hat{\mathbf{p}}^k)$$

or, equivalently, due to Eq. (10):

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

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

$$r_r \exp(3\hat{c}^k) = \hat{r} \exp(3\hat{c}_d^k) \quad (11)$$

where  $\hat{c}_d^k$  denotes the  $k$ -th eigenvalue of  $\text{dev}(\hat{\mathbf{C}})$ . The relevant interpretation of this result is given in the caption of Fig. 3.

The energy of the  $N_l$  interatomic bonds acting in  $d$  can then be expressed as a function  $U$  of the elementary, conformation tensor  $\mathbf{C}^{i,j}$  – more precisely, and for the value of this function to be an objective quantity, a function of the Euclidean norm of the elementary, conformation tensors and of some "crossed" invariants of the type  $\mathbf{C}^{i,j} : \mathbf{C}^{i,j+1}$  (e.g. [Spencer 1971]; [Boehler 1987]). No particular expression of the function  $U$  is given in this study. By contrast, it is postulated that there exists a state potential  $\mathcal{U}$  of average free energy of the interatomic bonds acting in  $d$ , depending only on the average conformation tensor  $\hat{\mathbf{C}}$ , and such that:

$$\mathcal{U}(\hat{\mathbf{C}}) = \frac{1}{N_l} U(\mathbf{C}^{i,j}, \dots, \mathbf{C}^{i,j} : \mathbf{C}^{i,j+1}, \dots) \quad (12)$$

Following the process presented in Section 2, the average internal forces tensor acting on the interatomic bonds belonging to  $d$  is then defined by:

$$\hat{\mathbf{F}} = \frac{1}{\hat{r}} \frac{\partial \mathcal{U}}{\partial \hat{\mathbf{C}}} \quad (13)$$

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

Note finally that directions of anisotropy  $\pm \mathbf{a}^n$  (those represented by the line segments in Fig. 2, for instance) could be simply taken into account by uniaxial tensors  $\mathbf{A}^n = (\pm \mathbf{a}^n) \otimes (\pm \mathbf{a}^n)$ , with 1 as the single non-zero eigenvalue. The tensors  $\mathbf{A}^n$  would then be new state variables on which the average free energy  $\mathcal{U}$ , see Eq. (12), would depend, via "crossed" invariants such that  $\mathbf{C}^{i,j} : \mathbf{A}^n$  (e.g. [Spencer 1971]; [Boehler 1987]). The immediate consequence of such a choice would be that the tensor of average internal forces,  $\hat{\mathbf{F}}$ , see Eq. (13), and that of average conformation,  $\hat{\mathbf{C}}$ , would not have the same eigenvectors, which is the main feature of anisotropy, at least in elasticity. Although the mechanical behavior of crystalline structure, such as the one illustrated in Fig. 3, is undoubtedly anisotropic, the directions of anisotropy  $\mathbf{A}^n$  will be ignored in the following sections, in order to focus attention on the main concept introduced in this study, namely the average conformation tensor of interatomic bonds.

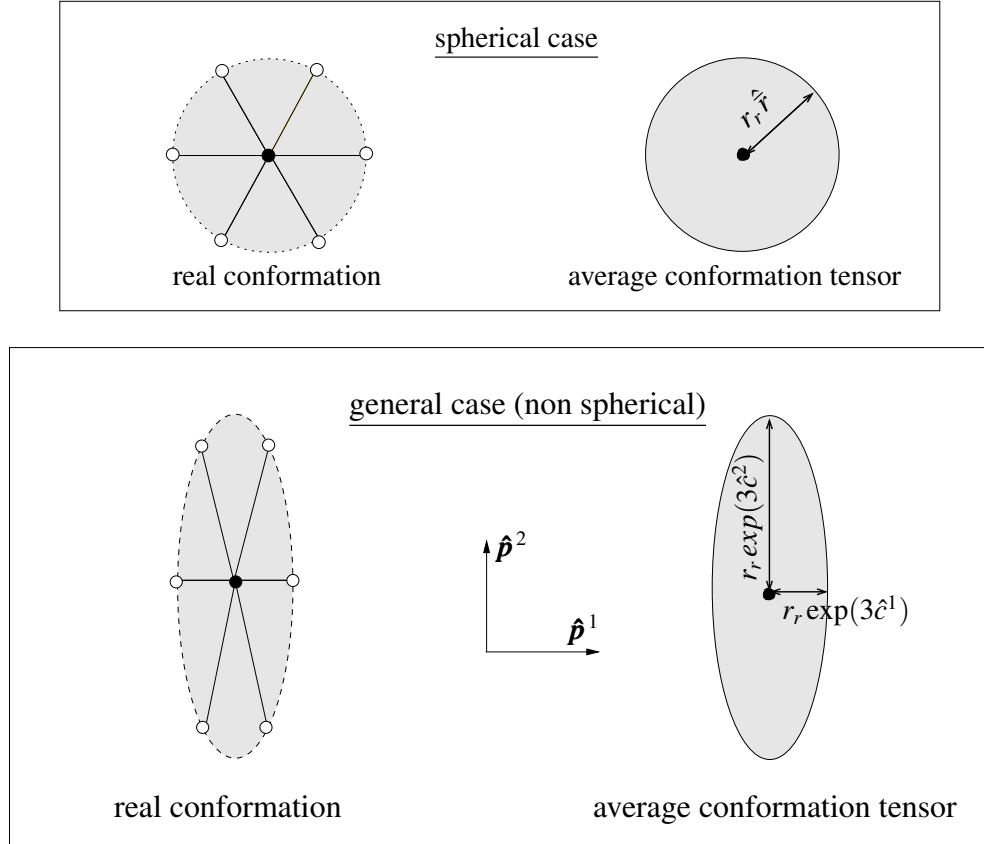


Figure 3: Interpretation of the eigenvalues and the eigenvectors of the average conformation tensor, here restricted to the 2D case, for the sake of simplicity. The real (discrete) conformations of the interatomic bonds are on the left part of the figure, their representation according to the average 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 neighbors (white dots in the real conformation) of a given atom (black dot). By contrast, it is possible to define the perimeter – the surface, in the 3D case – 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  $1/3 \ln(\hat{r})$ , the first neighbors of a given atom belong in average to the circle – the sphere, in the 3D case – with a radius  $\hat{r} = r_r \hat{r}$ . In the non spherical case (lower part of the figure), they belong to the ellipse with semi-axes  $r_r \exp(3\hat{c}^1)$  and  $r_r \exp(3\hat{c}^2)$  oriented along  $\hat{p}^1$  and  $\hat{p}^2$  – in the 3D case, to the ellipsoid with semi-axes  $r_r \exp(3\hat{c}^1)$ ,  $r_r \exp(3\hat{c}^2)$  and  $r_r \exp(3\hat{c}^3)$ , oriented along  $\hat{p}^1$ ,  $\hat{p}^2$  and  $\hat{p}^3$ .

## 4 Average conformation tensor of interatomic bonds, average internal forces tensor and Cauchy stress tensor: continuum approach

Let  $\mathcal{D}$  be the domain of the Euclidean space occupied by a pure substance in the solid state, considered as a continuous medium. The volume of  $\mathcal{D}$  is denoted by  $V$ . Since the substance is considered as a continuum – and since the number of atoms,  $N_a$ , as described in Section 3, is an extensive quantity –, an uniform field of density (per unit mass) of atoms can be defined, which is nothing more than the inverse of the atomic mass of the pure substance considered,  $\Delta_a = m_a^{-1}$ . Two other fields will have to be considered thereafter:

- the field of density (per unit mass) of interatomic bonds,  $\Delta_l$ ,
- the field of density (per unit mass) of  $\mathbf{C}$ -conformed interatomic bonds, namely, since  $\mathbf{C} = \ln(\bar{\mathbf{r}})\mathbf{N}$ ,  $\delta_l(\bar{\mathbf{r}}, \mathbf{N})$ .

Since the pure substance in the solid state considered in this section is supposed to be a continuous medium, these three fields are also continuous, which means that they are defined at any point  $P$  of  $\mathcal{D}$ . In the general case, however, and unlike  $\Delta_a$ , neither  $\Delta_l$ , nor  $\delta_l(\bar{\mathbf{r}}, \mathbf{N})$  is a uniform field. Denoting by  $N_l$  (resp. by  $n_l(\bar{\mathbf{r}}, \mathbf{N})$ ) the total number of active interatomic bonds (resp. of active,  $\mathbf{C}$ -conformed interatomic bonds) existing in  $\mathcal{D}$ , both these fields are still such that:

$$N_l = \int_V \Delta_l dm \quad ; \quad n_l(\bar{\mathbf{r}}, \mathbf{N}) = \int_V \delta_l(\bar{\mathbf{r}}, \mathbf{N}) dm \quad (14)$$

Like all the new quantities that have been defined so far,  $\delta_l(\bar{\mathbf{r}}, \mathbf{N})$  must be an objective quantity. A sufficient condition for this to be the case is that there exists an objective, symmetric, positive-definite tensor  $\mathbf{H}(\bar{\mathbf{r}})$ , such that:

$$\delta_l(\bar{\mathbf{r}}, \mathbf{N}) = \mathbf{H}(\bar{\mathbf{r}}) : \mathbf{N}$$

Hereafter in this study, it will be postulated that the tensor  $\mathbf{H}(\bar{\mathbf{r}})$  exists. Statistical considerations, however, can give some substance to this postulate. A Gamma distribution may therefore be considered, namely:

$$\varpi_k(\bar{\mathbf{r}}) = \frac{\mu_k^{\kappa_k}}{\Gamma(\kappa_k)} \bar{\mathbf{r}}^{(\kappa_k-1)} \exp(-\mu_k \bar{\mathbf{r}}) \quad \text{with} \quad \Gamma(\kappa_k) = \int_0^{+\infty} y^{\kappa_k} \exp(-y) dy$$

where the parameters  $\mu_k$  and  $\kappa_k$  are strictly positive. Such a statistical distribution is indeed such that the  $k$ -th eigenvalue of  $\mathbf{H}(\bar{\mathbf{r}})$  defined by:

$$H_k(\bar{\mathbf{r}}) = \alpha_k \varpi_k(\bar{\mathbf{r}}) \quad \text{with} \quad \alpha_k > 0 \quad (15)$$

is always positive, whatever  $\bar{\mathbf{r}} > 0$  is. It must be emphasized, however, that if the parameters  $\mu_k$ ,  $\kappa_k$  and  $\alpha_k$  really have a physical meaning, their values can be determined only by measurements at the nanoscale.

The full set of conformation tensors defines the conformation space,  $\mathbb{E}_c$ . Since the normalized length,  $\bar{\mathbf{r}} > 0$ , and the direction tensor,  $\mathbf{N}$ , are independent quantities, this space can be written:

$$\mathbb{E}_c = \mathbb{R}_+^* \times \mathbb{E}_N \quad \text{with} \quad \mathbb{E}_N = \{\mathbf{N} = (\pm \mathbf{n}) \otimes (\pm \mathbf{n}) \ ; \ (\pm \mathbf{n}) \cdot (\pm \mathbf{n}) = 1\} \subset \mathbb{R}^3 \times \mathbb{R}^3$$



where the volume of the direction space  $\mathbb{E}_N$  is half the surface of the unit sphere:  $V_N = 2\pi$ . At any one point  $P$  of  $\mathcal{D}$ , the density of interatomic bonds,  $\Delta_l$ , and that of  $\mathbf{C}$ -conformed interatomic bonds,  $\delta_l(\bar{r}, \mathbf{N})$ , are linked in the following way:

$$\Delta_l = \int_0^{+\infty} \int_{V_N} \delta_l(\bar{r}, \mathbf{N}) d\bar{r} dV_N$$

Through an approach similar to that followed in Section 3, the average conformation tensor of the interatomic bonds at any one point  $P$  of  $\mathcal{D}$  can then be defined:

$$\mathbf{\Gamma} = \frac{1}{\Delta_l} \int_0^{+\infty} \int_{V_N} \delta_l(\bar{r}, \mathbf{N}) \mathbf{C} d\bar{r} dV_N \quad (16)$$

Since  $\mathbf{C} = \ln(\bar{r})\mathbf{N}$  and  $\mathbf{N}:\mathbf{G} = 1$ , the trace of  $\mathbf{\Gamma}$  is:

$$\text{Tr}(\mathbf{\Gamma}) = \frac{1}{\Delta_l} \int_0^{+\infty} \int_{V_N} \delta_l(\bar{r}, \mathbf{N}) \ln(\bar{r}) d\bar{r} dV_N \quad (17)$$

which is the geometric mean of  $\bar{r} = r/r_r$ , as in the discrete case, see Eq. (10). The geometrical interpretation of the three eigenvalues  $\gamma^k$  – which are real since  $\mathbf{\Gamma}$  is symmetric – and the three eigenvectors  $\mathbf{P}^k$  – which are mutually orthogonal since  $\mathbf{\Gamma}$  is symmetric – of the average conformation tensor is also the same as in the discrete case, see Eq. (11) and Fig. 3. Since  $\Delta_l$ ,  $\bar{r}$ ,  $\mathbf{N}$  and  $\delta_l(\bar{r}, \mathbf{N})$  are objective quantities,  $\mathbf{\Gamma}$  is an objective quantity.

Following, once again, the process presented in Section 2, the free energy of a  $\mathbf{C}$ -conformed interatomic bond is characterized (at very first approximation here, that is to say, by omitting the "crossed" invariants, for the sake of simplicity) by a state potential of free energy  $u$ , depending only on  $\bar{r}$ , from which the average free energy of the interatomic bonds at any point  $P$  can be expressed, namely:

$$\hat{u} = \frac{1}{\Delta_l} \int_0^{+\infty} \int_{V_N} \delta_l(\bar{r}, \mathbf{N}) u(\bar{r}) d\bar{r} dV_N$$

It is next postulated that there exists a state potential of density (per unit mass)  $\Upsilon$  of average free energy of the active interatomic bonds existing at point  $P$ , depending only on the average conformation tensor  $\mathbf{\Gamma}$ , see Eq. (16), and such that:

$$\Upsilon(\mathbf{\Gamma}) = \Delta_l \hat{u} = \int_0^{+\infty} \int_{V_N} \delta_l(\bar{r}, \mathbf{N}) u(\bar{r}) d\bar{r} dV_N \quad (18)$$

The average internal forces tensor at any point  $P$ , actually being a density (per unit mass) of internal forces, is then given by, as in Section 3:

$$\mathbf{\Phi} = \frac{1}{\hat{r}} \frac{\partial \Upsilon}{\partial \mathbf{\Gamma}} \quad (19)$$

If the state potential of average free energy density  $\Upsilon$  depends only on the three invariants of  $\mathbf{\Gamma}$ , the quantity  $\Upsilon(\mathbf{\Gamma})$  is objective. Since  $\hat{r}$  is an objective quantity,  $\mathbf{\Phi}$  is thus also an objective quantity. The average internal forces tensor, 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 Eq. (19), on the basis of a simple dimensional analysis. It reads as follows:

$$\boldsymbol{\sigma} = \rho \hat{r} \boldsymbol{\Phi} = \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}} \quad (20)$$

It has been underlined previously that  $\Upsilon$  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  $\text{Tr}(\boldsymbol{\Gamma})$ ,  $\text{Tr}(\boldsymbol{\Gamma}^2)$  and  $\text{Tr}(\boldsymbol{\Gamma}^3)$ , the Cauchy stress tensor is then expressed by:

$$\boldsymbol{\sigma} = \rho \left( \frac{\partial \Upsilon}{\partial \text{Tr}(\boldsymbol{\Gamma})} \mathbf{G} + 2 \frac{\partial \Upsilon}{\partial \text{Tr}(\boldsymbol{\Gamma}^2)} \boldsymbol{\Gamma} + 3 \frac{\partial \Upsilon}{\partial \text{Tr}(\boldsymbol{\Gamma}^3)} \boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma} \right) \quad (21)$$

This equation shows, not surprisingly, 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 Eq. (20) or Eq. (21), and since  $\rho$ ,  $\hat{r}$  and  $\boldsymbol{\Phi}$  are objective quantities,  $\boldsymbol{\sigma}$  is an objective quantity. But, 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 Eq. (2):  $\mathbf{X}$  denoting some strain tensor,  $\boldsymbol{\Gamma} \neq \mathbf{X}$  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 Eq. (18) – such that  $\boldsymbol{\sigma} = \rho \partial \Upsilon / \partial \boldsymbol{\Gamma}$ . It must be recalled, however, that the stresses defined by Eq. (20) 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  $\mathbf{X}$  is also obtained by differentiating a state potential of free energy density, see Eq. (1). The two points of view, however, differ in an essential way: when a strain tensor  $\mathbf{X}$ , whatever it is, is intrinsically linked to a reference configuration (most of the time equal to the initial configuration), the average conformation tensor  $\boldsymbol{\Gamma}$  is independent of any reference configuration. In other words, the average conformation tensor is defined on the only current configuration of  $\mathcal{D}$  – in the sense that it is not linked to any Lagrangian gradient –, when a strain tensor is intrinsically linked to the transformation between the reference configuration and the current configuration of  $\mathcal{D}$ .

## 5 Thermodynamics and material derivative of the average conformation tensor of interatomic bonds

Like a strain tensor  $\mathbf{X}$  in the classical, thermodynamic approach to the modeling of the mechanical behavior of materials in the solid state, the average conformation tensor of interatomic bonds defined in Section 4,  $\boldsymbol{\Gamma}$ , is now considered as a state variable. By contrast, and unlike the material derivative of  $\mathbf{X}$ , 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 neighbors. 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 neighbors by active interatomic 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), the local expression of the first law of the Thermodynamics reduces to (e.g., [Coleman and Owen 1974]; [Garrigues 2007]):

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{D} \quad (22)$$

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  $\mathbf{D}$ , the rate of deformation tensor. The state potentials of the density of average internal energy,  $e$ , and of the average free energy,  $\Upsilon$ , are related by  $e = \Upsilon + sT$ , where  $s$  is the state function of the density (per unit mass) of entropy. An alternative, local expression for the first law of the Thermodynamics is then immediately deduced, namely:

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

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

$$\rho T \dot{s} = \boldsymbol{\sigma} : \mathbf{D} - \rho \frac{\partial \Upsilon}{\partial \boldsymbol{\Gamma}} : \dot{\boldsymbol{\Gamma}} \quad (23)$$

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

$$\omega = \rho T \dot{s} \geq 0 \quad \forall \boldsymbol{\Gamma}, \forall \mathbf{D} \quad (24)$$

where the quantifiers indicate that this inequality must always be fulfilled, that is, whatever the mechanical state,  $\boldsymbol{\Gamma}$ , and whatever the evolution,  $\mathbf{D}$ . From Eq. (23), Eq. (24) can be immediately rewritten:

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

or, equivalently, due to Eq. (20):

$$\omega = \boldsymbol{\sigma} : (\mathbf{D} - \dot{\boldsymbol{\Gamma}}) \geq 0 \quad \forall \boldsymbol{\Gamma}, \forall \mathbf{D}$$

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 (e.g., [Coleman and Gurtin 1967]). By definition, the mechanical behavior of a material is referred to as elastic when the intrinsic dissipation  $\omega$  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, whatever it is, cannot be objective (e.g., [Garrigues 2007]). As is also the case for  $\dot{\mathbf{\Gamma}}$ , which is necessarily the sum of an objective part  $\hat{\mathbf{\Gamma}}$ – directly linked to the material derivative of its eigenvalues which, on the contrary, are objective – and a non objective part  $\check{\mathbf{\Gamma}}$ – 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:

$$\omega = \boldsymbol{\sigma} : (\mathbf{D} - \dot{\mathbf{\Gamma}}) = \boldsymbol{\sigma} : (\mathbf{D} - (\hat{\mathbf{\Gamma}} + \check{\mathbf{\Gamma}})) = 0 \quad \forall \mathbf{\Gamma}, \forall \mathbf{D} \quad (25)$$

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

$$\hat{\mathbf{\Gamma}} = \mathbf{D} \quad (26)$$

It is not so immediate to give a mathematical expression for  $\check{\mathbf{\Gamma}}$ , knowing that its scalar product with  $\boldsymbol{\sigma}$  must always be equal to zero, see Eq. (25). The skew-symmetric part of the (Eulerian) velocity gradient,  $\mathbf{W}$ , is here helpful. It is such that, whatever the vector  $\mathbf{a}$ , the vector defined by  $\mathbf{W} \cdot \mathbf{a}$  is orthogonal to  $\mathbf{a}$ . Applied to the eigenvectors of  $\mathbf{\Gamma}$ ,  $\hat{\mathbf{p}}^k$  – which are the same as those of the Cauchy stress tensor in the isotropic case, see Eq. (21) –, this inherent property of the skew-symmetric tensors ensures that the following symmetric tensor ( $\gamma^k$  denote the eigenvalues of  $\mathbf{\Gamma}$ ):

$$\check{\mathbf{\Gamma}} = \sum_{k=1}^3 \gamma^k \left( (\mathbf{W} \cdot \mathbf{P}^k) \otimes \mathbf{P}^k + \mathbf{P}^k \otimes (\mathbf{W} \cdot \mathbf{P}^k) \right) \quad (27)$$

is such that its scalar product with  $\boldsymbol{\sigma}$  is always equal to zero, whatever the observer. Since  $\mathbf{W}$  is a non objective quantity,  $\check{\mathbf{\Gamma}}$  as defined by Eq. (27) is a non objective quantity. From Eq. (26) and Eq. (27), we immediately get that:

$$\dot{\mathbf{\Gamma}} = \mathbf{D} + \sum_{k=1}^3 \gamma^k \left( (\mathbf{W} \cdot \mathbf{P}^k) \otimes \mathbf{P}^k + \mathbf{P}^k \otimes (\mathbf{W} \cdot \mathbf{P}^k) \right) \quad (28)$$

is a condition for the intrinsic dissipation  $\omega$ , see Eq. (25), 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 Eq. (27) by any real number, another expression for  $\check{\mathbf{\Gamma}}$  is obtained which is also such that its scalar product with  $\boldsymbol{\sigma}$  is equal to zero. It may also be noted that, from the expression of the average conformation tensor in the orthonormal basis defined by its eigenvectors, namely:

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

which immediately gives the following form to the material derivative:

$$\dot{\mathbf{\Gamma}} = \sum_{k=1}^3 \dot{\gamma}^k (\mathbf{P}^k \otimes \mathbf{P}^k) + \sum_{k=1}^3 \gamma^k \left( \dot{\mathbf{P}}^k \otimes \mathbf{P}^k + \mathbf{P}^k \otimes \dot{\mathbf{P}}^k \right)$$

the objective part of  $\dot{\mathbf{\Gamma}}$ , according to Eq. (26) – and due to the fact that the material derivatives of the eigenvalues  $\gamma^k$  are objective –, is such that:

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

and the non objective part of  $\dot{\mathbf{\Gamma}}$ , according to Eq. (27) – and due to the fact that the material derivatives of the eigenvectors  $\mathbf{P}^k$  are non objective –, is such that:

$$\check{\mathbf{\Gamma}} = \sum_{k=1}^3 \gamma^k \left( (\mathbf{W} \cdot \mathbf{P}^k) \otimes \mathbf{P}^k + \mathbf{P}^k \otimes (\mathbf{W} \cdot \mathbf{P}^k) \right) = \sum_{k=1}^3 \gamma^k \left( \dot{\mathbf{P}}^k \otimes \mathbf{P}^k + \mathbf{P}^k \otimes \dot{\mathbf{P}}^k \right) \quad (29)$$

As defined by Eq. (27) or Eq.(29),  $\check{\mathbf{\Gamma}}$  is a traceless tensor, from which we immediately deduce that  $\text{Tr}(\dot{\mathbf{\Gamma}}) = \text{Tr}(\mathbf{D})$ . Furthermore, from the local expression of the law of conservation of mass, we also have  $\text{Tr}(\mathbf{D}) = -\dot{\rho}/\rho$ . Consequently:

$$\text{Tr}(\dot{\mathbf{\Gamma}}) = -\frac{\dot{\rho}}{\rho}$$

or, equivalently, due to Eq. (10) – where  $\mathbf{\Gamma}$  can be substituted to  $\hat{\mathbf{C}}$ , since the traces of these two tensors have the same interpretation, see Eq. (17):

$$\frac{\hat{r}}{r_r} = -\frac{\dot{\rho}}{\rho} \quad (30)$$

Denoting by  $\rho_0$  (resp. by  $\hat{r}_0$ ) the density (resp. the average distance between the atomic nuclei) at some initial time, Eq. (30) immediately gives:

$$\frac{\hat{r}}{\hat{r}_0} = \frac{\rho_0}{\rho}$$

which means that, if  $\rho \rightarrow 0$ , then  $\hat{r} \rightarrow \infty$ , and if  $\rho \rightarrow \infty$ , then  $\hat{r} \rightarrow 0$ . 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,  $\hat{r} \rightarrow \infty$ , because the distance between two atomic nuclei, that is to say, the length of an interatomic bond, is always finite in the solid state; the second one,  $\hat{r} \rightarrow 0$ , because the fusion of atomic nuclei is obviously not an elastic phenomenon.

## 6 An example of an elasticity model based on the conformation tensor

As noted previously, the average conformation tensor,  $\mathbf{\Gamma}$ , is not a strain tensor,  $\mathbf{X}$ , because its definition does not depend upon any Lagrangian gradient, see Eq.(16). However, from an experimental point of view, it is not without interest to seek for a relationship between  $\mathbf{\Gamma}$  – at least some of its components – and  $\mathbf{X}$ , whatever this strain tensor is: at the macroscopic scale, the tensor  $\mathbf{X}$  – at least some of its components – is indeed measurable when the tensor  $\mathbf{\Gamma}$  is only accessible by measurements at the nanoscale, see Eq. (15) and the following comment. 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

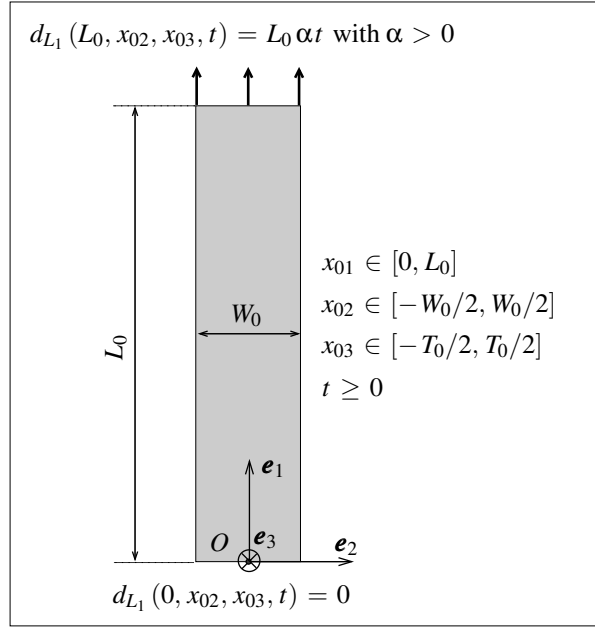


Figure 4: 2D representation of the gauge section of a flat tensile specimen. The Lagrangian displacement field is denoted by  $\mathbf{d}_L(\mathbf{x}_0, t)$ , where  $\mathbf{x}_0$  is the initial, position vector – for the observer defined by point  $O$  and the orthonormal basis  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$  – 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  $\mathbf{e}_2$  et  $\mathbf{e}_3$  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 gradient (Lagrangian) field of  $\mathbf{d}_L$  – and consequently, any strain field, whatever the considered strain tensor  $\mathbf{X}$  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  $\alpha t$  is nothing else than the axial strain of the gauge section, usually denoted by  $\varepsilon_{11}$  in the case of infinitesimal strains.

certain mathematical expression of the state potential of specific free energy, see Eq. (18).

Consider the gauge section of a flat tensile specimen whose dimensions are defined in Fig. 4. Due to the kinematic boundary conditions, the Lagrangian description of the displacement field of the points of the gauge section,  $\mathbf{d}_L$ , is simple – for the observer defined by point  $O$  and the orthonormal basis  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ , see Fig. 4. It reads:

$$\mathbf{d}_L(\mathbf{x}_0, t) = x_{01} \alpha t \mathbf{e}_1 + x_{02} g(t) \mathbf{e}_2 + x_{03} g(t) \mathbf{e}_3 \quad (31)$$

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  $\mathbf{d}_L$ , which defines a uniform field in the gauge section, the field of deformation gradient is immediately deduced, namely:

$$\mathbf{T} = \mathbf{grad}_L(\mathbf{d}) + \mathbf{G} = (1 + \alpha t)(\mathbf{e}_1 \otimes \mathbf{e}_1) + (1 + g(t))(\mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3)$$

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

$$\boldsymbol{\varepsilon} = \alpha t (\mathbf{e}_1 \otimes \mathbf{e}_1) + g(t) (\mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3) \quad (32)$$

From Eq. (31), the uniform field of the Eulerian velocity gradient  $\mathbf{v}$  is also deduced:

$$\mathbf{grad}_E(\mathbf{v}) = \frac{\alpha}{1 + \alpha t} (\mathbf{e}_1 \otimes \mathbf{e}_1) + \frac{\dot{g}(t)}{1 + g(t)} (\mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3)$$

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

$$\mathbf{D} = \mathbf{sym}(\mathbf{grad}_E(\mathbf{v})) = \mathbf{grad}_E(\mathbf{v}) \quad ; \quad \mathbf{W} = \mathbf{skw}(\mathbf{grad}_E(\mathbf{v})) = \mathbf{0}$$

The solution to the equation governing the material derivative of  $\boldsymbol{\Gamma}$ , see Eq. (28), 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):

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

There is no physical argument to claim that the initial state of average conformation,  $\boldsymbol{\Gamma}(0)$ , is zero. Quite the contrary, from Eq. (11) and the caption of Figure 3,  $\boldsymbol{\Gamma}(0) \neq 0$  describes a quite realistic physical condition, namely that on average the first neighbors 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  $\mathbf{P}_0^1$ ,  $\mathbf{P}_0^2$  and  $\mathbf{P}_0^3$  (here,  $\gamma_0^i$  denotes the  $i$ -th eigenvalue of  $\boldsymbol{\Gamma}(0)$  and  $\mathbf{P}_0^i$ , its  $i$ -th eigenvector; it can also be recalled that  $r_r$  is a reference length.) In the remainder of this section, however, and in order to facilitate the presentation of the main results, it will be assumed that  $\boldsymbol{\Gamma}(0) = \mathbf{0}$  – which is also a realistic condition, but very particular in the sense that on average the first neighbors 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 Eq.(32). Thus, in the case when  $\alpha t \ll 1$  and  $|g(t)| \ll 1$ , Eq. (33) simply becomes:

$$\begin{aligned}\Gamma_{11}(t) &= \varepsilon_{11}(t) \approx \alpha t \\ \Gamma_{22}(t) &= \Gamma_{33}(t) = \varepsilon_{22}(t) = \varepsilon_{33}(t) \approx g(t) \\ \Gamma_{ij}(t) &= \varepsilon_{ij}(t) = 0 \text{ when } i \neq j\end{aligned}\quad (34)$$

In other words, in the case of uniaxial tension restricted to the "small" strains, and for the observer defined by point  $O$  and the orthonormal basis  $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ , see Fig. 4,  $\mathbf{\Gamma} = \mathbf{\varepsilon}$ . In no way can this particular result be generalized, mainly because, as already mentioned,  $\mathbf{\Gamma}$  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  $\mathbf{\Gamma}$  are such that  $|\gamma^k| \ll 1$ , an expression of the average specific free energy of the interatomic bonds could be analogous to that underlying the very classical isotropic, linear elasticity model, namely:

$$\Upsilon(\mathbf{\Gamma}) = \frac{1}{\rho_0} \left( \frac{1}{2} \lambda (\text{Tr}(\mathbf{\Gamma}))^2 + \mu \text{Tr}(\mathbf{\Gamma} \cdot \mathbf{\Gamma}) \right) \quad \text{with } \mu > 0 \text{ and } \lambda > -\frac{2}{3}\mu \quad (35)$$

where  $\rho_0$  is the initial density, and where  $\lambda$  and  $\mu$  are analogous to the Lamé parameters. From Eq. (35), and in agreement with the general expression of the Cauchy stress tensor previously defined, see Eq. (20), we get :

$$\boldsymbol{\sigma} = \frac{\rho}{\rho_0} (\lambda \text{Tr}(\mathbf{\Gamma}) \mathbf{G} + 2\mu \mathbf{\Gamma}) \quad (36)$$

With the additional hypothesis that  $\rho/\rho_0 \approx 1$ , which is not inadmissible in the case of infinitesimal strains, Eq. (36) is therefore equivalent to the famous Hooke's law, where the infinitesimal strain tensor is replaced by the average conformation tensor  $\mathbf{\Gamma}$ . 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 Eq. (36) might well be non zero since the initial state of conformation has no reason to be zero – in Eq. (34), it has been assumed that  $\mathbf{\Gamma}(0) = 0$  only for the sake of brevity.

If one accepts, for "small" conformation variations, Eq. (36) 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. To highlight the fact that  $\mathbf{\Gamma}$  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  $\mathbf{\Gamma}_E(\mathbf{x}_t, t)$ , Eulerian field of the average conformation existing in the current configuration,  $\Omega_t$ , of the considered structure – as well as for the differential operators – such that  $\text{div}_E(\boldsymbol{\sigma})$ , Eulerian divergence of the stress field. The Eulerian field of the current position vector of the points of the considered structure is denoted by  $\mathbf{\Xi}_E(\mathbf{x}_t, t)$  (thus, trivially,  $\mathbf{\Xi}_E(\mathbf{x}_t, t) = \mathbf{x}_t$ ). The givens of the problem are as follows:

- the material parameters  $\mu > 0$  and  $\lambda > -(2/3)\mu$ ,
- the initial configuration – for any observer – of the considered structure,  $\Omega_0$ ,



- the initial fields of density  $\rho_0(\mathbf{x}_0)$  – e.g.  $\rho_0(\mathbf{x}_0) = \rho_0$  –, of average conformation  $\mathbf{\Gamma}_0(\mathbf{x}_0)$  – e.g.  $\mathbf{\Gamma}_0(\mathbf{x}_0) = \mathbf{0}$  –, and of Cauchy stresses  $\mathbf{\sigma}_0(\mathbf{x}_0)$  – e.g.  $\mathbf{\sigma}_0(\mathbf{x}_0) = \mathbf{0}$ ,
- the velocity field,  $\mathbf{V}_t(\mathbf{x}_t)$ , acting on the part  $\partial\Omega_t^V$  of the current boundary  $\partial\Omega_t$  of the structure, and the stress vector rate field,  $\mathbf{f}_t(\mathbf{x}_t)$ , acting on the part  $\partial\Omega_t^f$  of  $\partial\Omega_t$ ,
- the field of density (per unit mass) of body forces,  $\mathbf{f}^m(\mathbf{x}_t)$ , acting in  $\Omega_t$  – e.g.  $\mathbf{f}^m = \mathbf{0}$  or  $\mathbf{f}^m = \mathbf{g}$ , gravitational acceleration.

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

$$\begin{aligned}
\Omega_t &= \{\mathbf{\Xi}_E(\mathbf{x}_t, t) = \mathbf{x}_t\} \\
\dot{\rho}_E &= -\rho_E \text{Tr}(\mathbf{grad}_E(\dot{\mathbf{\Xi}})) \\
\dot{\mathbf{\Gamma}}_E &= \mathbf{sym}(\mathbf{grad}_E(\dot{\mathbf{\Xi}})) + \sum_{k=1}^3 \gamma_E^k \mathbf{sym}(\mathbf{skw}(\mathbf{grad}_E(\dot{\mathbf{\Xi}})) \cdot \mathbf{P}_E^k \otimes \mathbf{P}_E^k) \quad (37) \\
\mathbf{\sigma}_E &= \frac{\rho_E}{\rho_0} (\lambda \text{Tr}(\mathbf{\Gamma}_E) \mathbf{G} + 2\mu \mathbf{\Gamma}_E) \\
\mathbf{div}_E(\mathbf{\sigma}) + \rho_E \mathbf{f}^m &= \mathbf{0}
\end{aligned}$$

satisfying the following initial conditions ( $t_0 = 0$ ):

$$\begin{aligned}
\Omega_0 &= \{\mathbf{\Xi}_E(\mathbf{x}_0, 0) = \mathbf{x}_0\} \\
\rho_E(\mathbf{x}_0, 0) &= \rho_0(\mathbf{x}_0) \text{ in } \Omega_0 \\
\mathbf{\Gamma}_E(\mathbf{x}_0, 0) &= \mathbf{\Gamma}_0(\mathbf{x}_0) \text{ in } \Omega_0 \\
\mathbf{\sigma}_E(\mathbf{x}_0, 0) &= \mathbf{\sigma}_0(\mathbf{x}_0) \text{ in } \Omega_0
\end{aligned}$$

and satisfying the following boundary conditions ( $\mathbf{n}_E$  denotes the outward unit normal vector to  $\partial\Omega_t^f$ ):

$$\begin{aligned}
\dot{\mathbf{\Xi}}_E(\mathbf{x}_t, t) &= \mathbf{V}_t(\mathbf{x}_t) \text{ on } \partial\Omega_t^V ; \quad \dot{\mathbf{\sigma}}_E(\mathbf{x}_t, t) \cdot \mathbf{n}_E(\mathbf{x}_t, t) = \mathbf{f}_t(\mathbf{x}_t) \text{ on } \partial\Omega_t^f \quad (38) \\
\text{with } \partial\Omega_t^V \cap \partial\Omega_t^f &= \emptyset \text{ and } \partial\Omega_t^V \cup \partial\Omega_t^f = \partial\Omega_t
\end{aligned}$$

In Eq. (37), 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  $\mathbf{\sigma}$  –, 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 Eq. (35), and that on the boundary conditions, see Eq. (38). 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 Eq. (37), where both the symmetric and skew-symmetric parts of the velocity (Eulerian) gradient appear.

A final note should be made to well identify the area of validity of the previous problem. In this study, the average conformation tensor has been only defined for pure substances

in the solid state, in the restricted sense of substances composed of a single type of atoms. The pure metals are one example. They are often in the form of polycrystals, where each crystal is ideally defined by the periodic (at least initially) repetition of an elementary pattern: the unit cell. From the perspective here proposed, this unit cell is correctly depicted by an average conformation tensor of the interatomic bonds,  $\mathbf{\Gamma}_{el}$ , and the crystal, by a continuous medium where the (initial) conformation field is uniform and equal to  $\mathbf{\Gamma}_{el}$ . The average conformation of a crystal, not to be confused with its specific orientations (the crystallographic directions), is therefore physically relevant ; that of a polycrystal, however, as depicted by the conformation tensor alone, see Eq. (9) and Eq. (16), would be meaningless: the crystals of a given polycrystal have different crystallographic directions, which makes it impossible, for the polycrystal, to interpret the eigenvalues and eigenvectors of  $\mathbf{\Gamma}$  in the same way as in Eq. (11) and the caption of Figure 3. From that remark, it should be deduced that the problem defined by Eq. (37) is restricted not only to the "small", reversible variations of conformation, but to a "small", spatial scale, namely that of a crystal. It may still be added that this problem could be extended to polycrystalline structures, but on the express condition that the interfaces between crystals, that is, the grain boundaries, are precisely modeled.

## 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 that: i – as a state variable, the average conformation tensor of interatomic 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; ii – 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 interatomic bonds; iii – 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 neighbors, 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 neighbors. 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), (3), (4) and (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. Thus, the density, which has been related to the atomic mass in this paper, can be related in the same way to a "weighted" average of the atomic masses of the considered polyatomic material. A theoretical study, however, aiming to prove that the notion of the average conformation tensor of interatomic 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: i – which state variable(s) must be added to the average conformation tensor of interatomic bonds in a physically relevant model of the irreversible mechanical behavior (elastoplastic, for instance) of materials? ii – how is (are) the material derivative(s) of this (these) state variable(s), including that of the average conformation tensor of interatomic bonds, constrained by the Thermodynamics? If precise, rigorous answers can be given to these questions, the average conformation tensor of interatomic 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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