A texture tensor to quantify deformations

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Abstract Under mechanical deformation, most materials exhibit both elastic and fluid (or plastic) responses. No existing formalism derived from microscopic principles encompasses both their fluid-like and solid-like aspects. We define the *statistical texture tensor* to quantify the intuitive notion of stored deformation. This tensor links microscopic and macroscopic descriptions of the material, and extends the definition of elastic strain.

Keywords Strain, Connected network, Elasticity of disordered media, Deformation and plasticity

A typical mechanical experiment applies a given macroscopic distortion to a test sample and measures the resulting macroscopic force exerted by the material, or *vice versa*. The goal is to find the constitutive equation, which relates the macroscopic stress tensor to an independent descriptor of the material's response. We know the relevant descriptor to use for two extreme cases, elastic solids

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and isotropic fluids: the gradient of the displacement and the velocity field, respectively.

While stress is unambiguously defined [1,2], strain admits more than one definition. Classical linear (or even non-linear) elasticity operationally defines the strain by comparing the current microscopic state to a fixed microscopic reference state [3–5]. But most materials, having both an internal structure which stores elastic energy and the flexibility to allow rearrangements, lie between ideal fluids and purely elastic solids. Not only do we lack their exact constitutive relations, we do not know what descriptors apply.

In this paper we propose an operational definition of the deformation which we can measure in experiments and simulations in terms of averages of microscopic quantities: the *statistical texture tensor*, a state function of the material. Its variations measure the elastic strain of an object under arbitrary deformations, without requiring the microscopic details of a reference state.

Unlike Ref. [6] which starts from a coarse grained mass density, which is appropriate for granular materials, we consider a network structure. Our generic material is a network of sites connected by links, which can detach from and reattach to other sites (Fig. 1). Site and link definitions depend on the material:

(i) In cellular patterns, a site is the meeting point of cells. Two sites connect if their cells share an edge. This situation applies, for instance, to grain boundaries in crystals [7], compact 2D or 3D aggregates of biological cells, or Voronoi tesselations

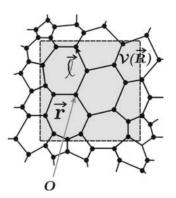


Fig. 1. A network of interconnected sites. The representative volume element $\mathcal V$ at position $\vec R$ is a square in two dimensions; its volume is V. Microscopically, $\vec r$ is the position of a site which here has three links (unoriented vectors $\vec \ell$)

- (ii) If links are physical objects, sites need not be. In liquid foams, links are bubble edges, while sites are the vertices where they meet. In gels of polymers, links are macromolecules; sites are knots.
- (iii) If sites are undeformable objects, as in hard granular materials, they link if their separation is less than a cut-off distance. Since such a cut-off is arbitrary, it must be chosen consistently throughout the analysis.
- (iv) When two sites exert a force on each other, they are linked. This is the case, e.g., for atoms or molecules in crystalline and amorphous solids, or deformable granular materials. We then have to specify a cut-off on their interaction force (Cauchy scheme): again, such an arbitrary cut-off must be chosen consistently.

Note that, even in cases (ii) and (iv), the strain remains purely geometric and does not depend explicitly on stresses and forces, as seen in 3D foams where the films determine the stress [8] while the edges determine the statistical strain.

For simplicity, we consider only point-like isotropic sites, i.e. the average link length is much larger than the site size, and the unstressed material is mesoscopically isotropic [9]. Neither restrictions is essential: we could relax them by extending our definitions.

At the microscopic level, we describe our material by the positions $\{\vec{r}_s\}$ of the sites $\{s\}$ in a d-dimensional space (Fig. 1). The $topology\ \mathcal{T}$ is the list of all pairs (s,s') of sites connected by a link $\vec{\ell} = (\ell_x,\ell_y,...) = \vec{r}_{s'} - \vec{r}_s$. The topology changes when perturbations create or destroy a link or a site.

A continuous description interpolates between this microscopic level of description and a macroscopic description in terms of the shape and size of the network boundaries. We define an intermediate mesoscopic level (Fig. 1). We cut the network into representative volume elements, $\mathcal{V}(\vec{R})$ of volume V, at position \vec{R} : small enough that their properties are constant over the box; but large enough that each piece contains enough links to compute statistical properties and average out microscopic details. In each volume element we define all statistical quantities as averages over all links in $\mathcal{V}(\vec{R})$. The number of neighbours of each site must be much smaller than the number of links in $\mathcal{V}(\vec{R})$. We thus require that the topology remains "short-range;" while the neighbours s' of a site s may change, their number must remain bounded.

Our fundamental definition is the texture tensor:

$$\overline{\overline{M}}(\vec{R}) \equiv \left\langle \vec{\ell} \otimes \vec{\ell} \right\rangle. \tag{1}$$

Here $(\vec{\ell} \otimes \vec{\ell})_{ij} = \ell_i \ell_j$ is the "dyadic" (or "outer" or "tensor") product. $\overline{\overline{M}}$ is symmetric, and has positive eigenvalues. $\overline{\overline{M}}$ occurs in many different physical contexts: the Steiner Tensor [10–12], order parameters of nematics [13], molecular moments of inertia ([14] p. 116–119), or textures of granular materials [15]. The texture tensor quantifies our mental image of a network; large eigenvalues correspond to directions of stretching (Fig. 2).

This definition (1) encompasses all materials where a mesoscopic scale exists, *i.e.*, most cases. It requires that a thermodynamic limit exists for all extensive and intensive

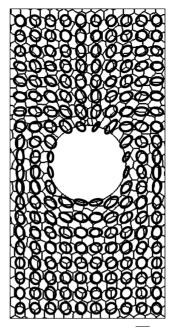


Fig. 2. Texture tensor \overline{M} (eq. 1) superimposed on a snapshot of a simulated two-dimensional foam. The foam flows steadily from left to right around a fixed round obstacle. We calculate the texture tensor over a box almost as small as the bubble size, by averaging over 50 successive images. The texture tensor is symmetric with two positive eigenvalues. We represent it as an ellipse, with the long axis (resp. small axis) proportional in length to the largest (resp. smallest) eigenvalue and pointing along the corresponding eigenvector. We see compression deformation in front of the obstacle, and stretching behind it

quantities, *i.e.* statistics on larger volumes decrease the relative amplitude of fluctuations (these microscopic fluctuations might remain visible on the scale of the sample size if the sample is small [16] or if the lattice is ordered [17]). We assume no correlations between the volume elements, which we must check. Materials that display networks of forces, avalanches or fractures thus require careful treatment. For materials in ergodic steady flow, time averages also reduce fluctuations and the network acts as a continuous medium down to scales as small as the average link length (Fig. 2).

If each region has an isotropic reference state [9], then $\overline{\overline{M}}_0 = M_0 \, \overline{\overline{I}}_d$, where $\overline{\overline{I}}_d$ is the identity tensor in d dimensions. All its relevant information lies in the scalar $M_0 = \left<\ell_0^2\right>/d$, i.e. in the mean squared link length in this state [18].

We now define the "statistical strain" \overline{U} as:

$$\overline{\overline{U}}\left(\vec{R}\right) \equiv \frac{\log \overline{\overline{M}} - \log \overline{\overline{M}}_0}{2},\tag{2}$$

where the tensor $\log \overline{\overline{M}}$ has the same axes as $\overline{\overline{M}}$ but eigenvalues equal to the logarithm of those of $\overline{\overline{M}}$.

Eq. (2) is operational: \overline{U} quantifies the deformations visible locally in each region of an image, such as extension, compression, shear, or dilation (Fig. 2). $\overline{\overline{U}}$ also satisfies other requirements for the definition of strain. It is

invariant under rotation, translation and transposition of indices. It is a true function of state; it depends explicitly only on the current state and the reference state, not on the detailed history of the material. It is mesoscopic; it reflects only statistically significant features of the network. Its definition (eq. 2) accommodates topological changes and thus the plastic regime.

Finally, we prove that whenever the classical definition of the strain tensor applies, it coincides with our statistical strain $\overline{\overline{U}}$. Under an arbitrary elastic deformation from an initial, equilibrium, isotropic state to a final state, we have:

$$\overline{\overline{U}} = \frac{1}{2} \left(\overline{\overline{w}} + \overline{\overline{w}}^t \right) + O\left(w^2 \right). \tag{3}$$

Here we do not make any assumptions about the microscopic displacements. The displacement field $\vec{u}(\vec{R})$ is the difference between states in the region $\mathcal{V}(\vec{R})$, initially at position \vec{R} . When $\vec{u}(\vec{R})$ is differentiable, the distortion tensor $\overline{\overline{w}} = [\vec{\nabla} \otimes \vec{u}]^t = \partial u_i/\partial r_j$ quantifies the deformation from initial to final state. The proof goes as follows:

As a first step, we have to prove that the average over the surface element $\vec{n}dS$ (or line elements, in two dimensions), denoted $\langle . \rangle^{\vec{n}}$, of any function $g(\vec{\ell})$ of the links which actually cross this surface, relates to its bulk average, denoted $\langle . \rangle$, as:

$$\forall \vec{n}, \quad \langle g \rangle^{\vec{n}} \langle \ell_i \rangle \, n_i = \langle g \ell_i \rangle \, n_i. \tag{4}$$

Here $\langle \ell_j \rangle$ depends on the orientation chosen for the link; it must be chosen consistently along the surface, for instance along the orientation of \vec{n} . On the other hand, if g is an odd function of the link $\vec{\ell}$, i.e. $g(-\vec{\ell}) = -g(\vec{\ell})$, then the quantity $g(\vec{\ell})\vec{\ell}$ does not depend on the arbitrary orientation choosen for the link; in that case, $\langle g\ell_j \rangle$ does not depend on \vec{n} , so that we can omit \vec{n} in what follows.

To prove this first step, eq. (4), we remark that for any elementary section $d\vec{S} = \vec{n}dS$ of C, oriented by the unit vector \vec{n} , the probability for a link to cross $d\vec{S}$ is proportional to:

$$\rho \vec{\ell} \, \cdot \vec{n} \, dS \, P(\vec{\ell} \,) \, d^3 \vec{\ell},$$

where ρ is the average density of links, and P is the probability distribution function of the links $\vec{\ell}$. Hence the sum of g taken over all links crossing $d\vec{S}$ is: $\sum_{\vec{dS}} g(\vec{\ell}) = \rho \iiint g(\vec{\ell}) \vec{\ell} \cdot \vec{n} \, dS \, P(\vec{\ell}) \, d^3 \vec{\ell}$. In particular, with g = 1 we obtain the number of links crossing $d\vec{S}$:

$$\rho \iiint \vec{\ell} \cdot \vec{n} \, dS \, P(\vec{\ell}) \, d^3 \vec{\ell}.$$

Combining both proves eq. (4).

At this point, it is interesting to apply eq. (4) to the forces. By definition [3,4], the stress $\overline{\overline{\sigma}}$ is the tensor such that, $\forall \vec{n}$:

$$\sigma_{ij}n_j\,dS = \sum_{\vec{dS}} \tau_i,$$

where $\vec{\tau}$ is the tension (force) supported by the link $\vec{\ell}$. With $g(\vec{\ell}) = \tau_i$, eq. (4) yields:

$$\overline{\overline{\sigma}} = \rho \langle \vec{\tau} \otimes \vec{\ell} \rangle$$
,

providing a statistical interpretation of the stress tensor as an average over all links [8].

Now, we can prove eq. (3). By the definitions of \vec{u} and $\overline{\overline{w}}$, we can write:

$$\begin{split} \left\langle \delta \vec{\ell} \right\rangle^{\vec{n}} &= \left\langle \delta \vec{r} \right\rangle^{\vec{n}} (\vec{R} + \left\langle \vec{\ell} \right\rangle^{\vec{n}}) - \left\langle \delta \vec{r} \right\rangle^{\vec{n}} (\vec{R}) \\ &= \vec{u} (\vec{R} + \left\langle \vec{\ell} \right\rangle^{\vec{n}}) - \vec{u} (\vec{R}) \\ &= \overline{\vec{w}}^t \left\langle \vec{\ell} \right\rangle^{\vec{n}} + O\left(w^2\right). \end{split} \tag{5}$$

With $g(\vec{\ell}) = \delta \ell_i$, eq. (4) yields:

$$\left\langle \delta \vec{\ell} \otimes \vec{\ell} \right\rangle = \left\langle \delta \vec{\ell} \right\rangle^{\vec{n}} \otimes \left\langle \vec{\ell} \right\rangle,$$

which inserted into eqs. (1) and (5) yields:

$$\overline{\overline{M}} = \overline{\overline{M}}_0 + \overline{\overline{M}}_0 \overline{\overline{w}} + \overline{\overline{w}}^t \overline{\overline{M}}_0
= M_0 \left(\overline{\overline{I}} + \overline{\overline{w}} + \overline{\overline{w}}^t \right) + O\left(w^2\right).$$
(6)

Combining eqs. (2) and (6) proves eq. (3).

Hence the statistical strain $\overline{\overline{U}}$ coincides with the elastic strain. Note that in the (rare) cases where the microscopic displacements are affine, then $\vec{\ell} = (\overline{\overline{I}} + \overline{\overline{w}}^t) \ \vec{\ell}_0, \ \forall \vec{\ell}$. This statement is very strong since each link (and not only the average) obeys eq. (5); in this case, eq. (3) is easier to demonstrate.

In summary, we have proposed a statistical characterization of deformation. It averages the microscopic details of the current pattern and of the reference state, to keep only the physical features statistically relevant at large scales. Hence, different microscopic configurations which are statistically identical correspond to the same statistical strain (for instance, ductile metals like soft steel or aluminium have almost unchanged Young's modulus even much beyond their yield strain [19]) so, although different applied strains correspond to different microscopic structures, they have the same statistical strain, the same static stress and the same mechanical response for any physically reasonable static constitutive relation. Or, in a steadily flowing material, \overline{U} is constant; we thus provide an operational definition for the thermodynamic stored strain that Porte et al. [20] introduced to allow a theoretical description of shear-induced phase transitions.

This definition invites re-analysis of existing data, as well as experimental, numerical and theoretical tests. In a companion paper we have successfully performed such tests on an experiment which forces a two-dimensional foam to flow through a small constriction [21].

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