AN APPROACH TO DEFORMATION THEORY BASED ON THERMODYNAMIC PRINCIPLES

FALK H. KOENEMANN
Im Johannistal 19
D-52064 Aachen, Germany
peregrine@t-online.de

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The Cauchy stress theory has been shown to be profoundly at variance with the principles of the theory of potentials. Thus, a new physical approach to deformation theory is presented which is based on the balance of externally applied forces and material forces. The equation of state is generalized to apply to solids, and transformed into vector form. By taking the derivatives of an external potential and the material internal energy with respect to the coordinates, two vector fields are defined for the forces exerted by surrounding at the system, subject to the boundary conditions, and vice versa, subject to the material properties. These vector fields are then merged into a third one that represents the properties of the loaded state. Through the work function the force field is then directly transformed into the displacement field. The approach permits fully satisfactory prediction of all geometric and energetic properties of elastic and plastic simple shear. It predicts the existence of a bifurcation at the transition from reversible to irreversible behavior whose properties permit correct prediction of cracks in solids. It also offers a mechanism for the generation of sheath folds in plastic shear zones and for turbulence in viscous flow. Finally, an example is given how to apply the new approach to deformation of a discrete sample as a function of loading configuration and sample shape.

Keywords: elasticity, thermodynamics, anisotropic change of state, pure shear, simple shear

1. Introduction

A change of paradigmata occurred in natural philosophy around 1790-1810, initiated by Young, Lagrange, and Carnot. Before, the theoretical development in physics was mainly driven by the study of celestial phenomena which can be understood by Newtonian concepts – that is, a need to consider energy as a physical quantity emerged only very slowly. After that, energetic thinking became prevalent, as evidenced by the approach of Lagrange, the equation of Hamilton, and the first law of thermodynamics by Mayer, Joule, and Helmholtz. The result was the recognition of two fundamental classes of physical processes in the mid-19th century:

- during a conservative process, the energy of the system under discussion is invariant;
- during a non-conservative process, the energy of the system is a variable.

The latter class again permits the recognition of two subclasses:

- during a reversible process, no entropy is produced, and all the work done on the system may be recovered;
- during an irreversible process, entropy is produced, hence it is impossible to reach the original state unless additional work is done.

Continuum mechanics is still a child an older period; the first steps were made in the mid-18th century. The theories of stress and strain developed side by side, but curiously independent of one another. Characteristically even for most recent textbooks,

the theory of strain – the effect – is discussed before the cause – stress – after which the material laws are mentioned.[1-4] This appears to be the inverse order of priorities. Textbooks on thermodynamics start with the equation of state which is the material law for an ideal gas, continue with changes of state of which stress is but one form, and the effects are the solution for which no extra theory is then required. Deformation has been merely understood as a topological mapping, not as a physical process. To illustrate this point, the compatibility problem in continuum mechanics – that two separate points in the initial state must not coincide after a deformation – cannot occur in reality; it follows from Boyle´s law that two points can coincide only at the expense of infinite work.

Much of Euler´s work was done in the 1740´s; the equations that continue to govern the current understanding of continuum mechanics were published 30 years later.[5] Before elastic deformation could be perceived as an anisotropic change of the energetic state, energy had to be recognized as a concept different from force – by Young in 1787, – the equation of state had to be completed – by Gay-Lussac in 1808, – and the concept of the thermodynamic system that is distinguished from its surrounding, had to be established in the early 19th century. It has been noted before that the theories of continuum mechanics and of thermodymanics are not consistent with one another.[6] The backbone of classical physics in general is the theory of potentials.[7] It follows from this theory that an approach for a theory for a conservative process is to be derived starting with the Laplace equation, whereas an approach for changes of state, which includes all of continuum physics, is governed by the Poisson equation,[8] – except the Cauchy stress theory and continuum mechanics. It has already been shown that the derivation of the stress tensor by Cauchy is at variance with the Gauss divergence theorem.[9]

The transformation of the unloaded to the loaded elastic state is unquestionably a non-conservative, reversible process. However, nothing in the Euler-Cauchy theory of stress and deformation permits such a conclusion. To the contrary, virtually all the conceptual tools of the Euler-Cauchy theory – use of an equation of motion vs. an equation of state; use of the inertial mass density vs. the molar density; use of a Newtonian force $\mathbf{f} = m\mathbf{a}$ vs. an energy flux $\mathbf{f} = \mathbf{e}_i \partial U/\partial x_i$, treat stress and deformation as a conservative process. For example, the Euler-Cauchy theory does not permit the definition of a non-zero elastic potential for a volume-neutral deformation. The particular form of the First Law of thermodynamics which is given in the literature on elasticity, is incompatible with the nature of the First Law, in fact it turns the latter upside down.[10, 11] The recognition of a misconception of such proportions renders the Euler-Cauchy theory invalid.

The only possible conservative deformation process is volume-constant equilibrium flow of an ideal gas, but then, no elastic potential builds up. Elastic deformation is a reversible change of state. The simplest perceivable elastic deformation is the volume change of a gas, hence the most primitive deformation law is Boyle's law. Viscous and plastic flow are irreversible. For a more in-depth discussion of the Euler-Cauchy approach see Ref.9-12.

In this paper, a new approach to time-independent, reversible elastic deformation of solids and the properties of the loaded state is presented. Deformation is understood not as a change of shape in the first place, but as a change of state, and energetic rather than

geometric considerations provide the most stringent constraints. There is no resemblance between the Euler-Cauchy theory and this one which is derived from the theory of thermodynamics: a vector field of forces is developed from a scalar potential field; after a discussion of the material law, the kinematics of deformation is explained using pure shear as an example; the result is the displacement field.

2. Symbolic Terminology

T, **M**, **F**	tensors	**f**, **m**, **r**, **s**, **v**	vectors
I	identity tensor	**n**, **t**	unit vectors
T_{ij}, F_{ij}	tensor components	r_i	vector components
P, V, H, U	scalars, state functions	f, r	vector magnitudes
P, Q	points	α, γ, θ	angles

3. General Remarks

If a theory has dominated a field of science for a long time it has shaped the mind of its user considerably, to the effect that he does not even realize it any more. To get rid of such a concept in the back of ones´s head is more difficult than to store a new concept in an unpreconditioned mind. There is no easy transformation matrix which turns the insights according to the old approach into useful knowledge about the new one. This section is written for the reader who is familiar with the Euler-Cauchy theory, and hence not familiar with potential theory.

1. The classical question in deformation theory is the stress-strain relation. However, it is known from experiments that pure and simple shear require different amounts of work per unit strain; in the elastic field, simple shear costs more than pure shear, in the plastic field it costs substantially less. Therefore strain in the sense of the strain tensor ε is not a thermodynamic state function, and the concept of strain is of limited value. Displacement is sensitive to these differences. In this paper, a cause-effect relation is developed between a force field and the displacement field.

The classical question in potential theory is the search for sources and sinks. Any system of matter that is not in its zero potential state, is a source or a sink of fluxes, or both. The fluxes may be mechanical forces. The present approach is that of thermo-dynamics. It considers the cause of a deformation: external forces controlled by external boundary conditions; to these the system acts as a sink. Also, a given field of external forces will produce a state of deformation that varies due to the chosen material properties; that is, the application of the external field will *evoke* a material force field the properties of which represent the material properties; to these material forces the system acts as a source. The two fields are independent in nature, but together they result in a third force vector field which combines the properties of both. A work function is derived from the state function; with its help, the displacement field is calculated such that the geometric properties of force field and displacement field are identical.

2. The term *stress* is so strongly occupied by a concept which is here taken to be invalid that it appears better to avoid it altogether. In this essay, the term *loaded state* will be used. It is, admittedly, very tempting to apply the term stress to the force field $\mathbf{f}_{\text{total}}$ which has the same properties as the displacement field. However, that field is a vector field and not a tensor quantity. Perhaps it is better to leave *stress* to the shrinks for further abuse, and continue with proper physics.

3. The Euler-Cauchy approach started with an equation of motion; this one starts with an equation of state. An equation of motion applies to the mechanics of discrete bodies in free space, but not to changes of state since a reversible thermodynamic change of state is time-independent. Instead, the common state function $PV = nRT$ is transformed into vector form, using $\mathbf{f} = \mathbf{e}_i \partial U/\partial x_i$ instead of $\mathbf{f} = m\mathbf{a}$ as the force definition.

4. The Euler-Cauchy approach used a continuity approach that supposedly transformed a region occupied by mass into a continuum of mass points. That concept is ruled out by the principles of potential theory because a volume distribution cannot be reduced to a point source. The approach proposed here uses the proportionality of mass and potential in a given state, $P = \partial U/\partial V$, to arrive at the elastic potential, or the loaded state or the work done *per unit mass* (n in $PV = nRT$ is finite). The existence of the continuum of mass is a precondition. Discontinuous conditions, such as near surfaces between the interior of the body and the exterior free space, change the local boundary conditions. An example will be given at the end of this paper.

5. Much in the understanding of elasticity relates to the work done in achieving a deformation. The simple expression $\nabla^2 U = \varphi$ is handy, but it is an implicit statement that only normal vector components have an effect on the energy U of the system. This is correct for heat flow because heat always flows radially, and for mechanical forces if the state of loading and the material are both isotropic, such as in the compression of a gas. In anisotropic states of loading, the properties of the tensor term are insufficient because there are bonds in solids, and shear forces do work.

6. None of the concepts in continuum mechanics that can be traced back to Euler have been found to be helpful. Euler's definition of normal force $\mathbf{f}\cdot\mathbf{n}$ and shear force $\mathbf{f}\times\mathbf{n}$ are defined relative to the plane on which they act. Newton defined normal and rotational force relative to the radius vector with which they interact, $\mathbf{f}\cdot\mathbf{r}$ and $\mathbf{f}\times\mathbf{r}$. Euler's definitions cannot be transformed into those of Newton; in this paper Newton's principles are observed.

7. The Newtonian definition of pressure $P = f/A$ cannot be used in this context because of the scale-dependence of the ratio f/A for closed surfaces.[9, 11] The thermodynamic definition $P = U/V$ is a scalar, the energy density, it is by definition scale-independent, hence it is more fundamental; it is a statement of the most profound principle in potential theory, the proportionality of mass and potential in a given state. If an intensive physical quantity is a scalar, it does not have properties that vary with direction. Hence is implied that it is isotropic, providing tight constraints on its discussion; this is not at all evident from f/A.

8. The inertial mass density ρ [g/cm^3] cannot be used to define an equation of state in thermodynamics. The thermodynamic mass density mol/V is not a state function by definition; it may be used as such for isotropic loading (the common boundary condition

in standard thermodynamics), but not for anisotropic loading: for example, in a volume-neutral deformation the internal energy U is changed whereas mass is constant.

9. Spatially extended bodies necessarily have a specific shape which strongly influences the particular form of the equilibrium conditions in Newtonian mechanics. In the Euler-Cauchy theory of continuum mechanics the shape, including the radius, was lost through the Cauchy continuity approach which, however, violates an existence theorem in potential theory.[11, 12] The shape of the region bounded by the surface integral in the divergence theorem is arbitrary only if the surface does not pass through mass. This is not the case in continuum physics; the shape is therefore of profound importance because the surface-volume ratio per unit mass is not arbitrary. Newton's radius $\mathbf{r}$ (as in $\mathbf{f}\times\mathbf{r}$ in the consideration of rotational equilibrium) is here equated with the zero potential distance of potential theory, and the shape of the thermodynamic system represents the material properties. Throughout this paper the material is assumed to be isotropic.

Model calculations are initially restricted to two dimensions for simplicity. Calculations are commonly given in vector notation and in algebraic terms, e.g.,

$$\int \mathbf{f}\times\mathbf{r}\, d\theta = \int \sin\theta\cos\theta\, d\theta$$

where the LHS vector operations explain what is being done, and the scalar RHS shows how it is done. They are related to one another by an equation sign = rather than a proportionality sign $\propto$ because it made much easier reading. The equation sign implies that a proportionality constant on the RHS has unit magnitude.

4. The Thermodynamic System in Euclidean Space

Any mass is associated with a potential. The gravitational potential Z is invariant with respect to the inertial mass m. The inertial mass density is $dm/dV = \rho$, where any inertial mass differential dm is associated with a gravitational potential dZ, such that the potential $Z \propto m = \rho\int dV$. The same holds for a thermodynamic potential U except that its magnitude per mass may be a variable. In a given state, $dU \propto dn$ where n is the number of mol (the thermodynamic mass is dimensionless). The energetic density per unit mass is then $dU/dV = P$, or in integrated form $U/V = P$ where the mass is proportional to both U and V. Note that mass is a variable in this integration. Just as ρ may be understood as the density of inertial mass per unit volume, P is the energy density, or thermodynamic potential U per unit mass. U is then finite.

In the reference state U_0 we have $PV = nRT$. An infinitesimal change of state requires the additional energy dU. Of course, the nature of this dU at constant n is very different from that of $dU \propto dn$ above. In order to consider infinitesimal changes of state, a system of finite mass and volume is a prerequisite – a thermodynamic system – which is associated with its self-potential.

In order to define the work done on a point P_0, a reference point Q must be chosen such that $Q \neq P_0$. The choice is arbitrary and may be defined to the convenience of the problem (Ref.7, p.53, 63; Ref.13). The distance $Q \to P_0$ is the zero potential distance r. Consider a discrete body in freespace. If the body is contained in a region V such that

the surface A of V does not touch the body, the mass may be thought to be concentrated at a point in V. The mass may then be considered a point source, and $\int \nabla \cdot \mathbf{f}\, dV = \kappa = const$ is independent of the limits of integration. In such a case, r is commonly chosen to be infinite, such as in gravity problems since the gravitational potential reaches zero at infinity. However, in continuum physics that option is not possible since mass and potential are proportional, and $\kappa \propto V$. Since mass is evenly distributed over the region enclosed by the thermodynamic system and in the immediate surrounding, it represents a *distributed source* (Ref.7, p.156). The potentials of distributed source problems are commonly logarithmic. In such a case the zero potential distance may be finite, it is then by convention assigned unit magnitude. In the current context, the zero potential distance is interpreted to be the radius of the thermodynamic system r. (In Hooke's law the zero potential distance is the length l_0 of the spring. In Cauchy's stress theory the zero potential distance is allowed to vanish identically which is not permissible; Ref.7, p.63).

In thermodynamics, the properties of substances are given in a standard state (P^*, V^*, T^*) which may then also serve as a zero potential state (the unloaded state), and a change of the pressure to $\pm\infty$ requires infinite work. The distance term r is the one-dimensional equivalent of the volume of the mass n to which the equation of state $PV = nRT$ is scaled. For solids which have a non-zero density in a vacuum, the zero potential state is then defined by $P^* = P_{\text{int}}$. A deviation from r_0 indicates a change of state. In the discussion of pure shear deformation, r_0 is set to be invariant with respect to direction, i.e. the shape of the thermodynamic system is assumed to be a sphere because it minimizes the surface-volume ratio. The material is therefore defined to have isotropic properties. In the discussion of simple shear, additional constraints require another shape.

Consider the divergence theorem for an isotropic loading state, such that only normal (radius-parallel) forces need to be taken into account,

$$\int \mathbf{f} \cdot \mathbf{n}\, dA = \int \nabla \cdot \mathbf{f}\, dV = \kappa\,, \tag{1}$$

where $\mathbf{n}$ is a unit vector normal to A. Consider forces as an energy flux, $\mathbf{f} = \mathbf{e}_i \partial U/\partial x_i$. The surface A is closed to envelop a volume element $\int dV$; the forces are exerted by the mass in the element against the surrounding, or vice versa. At similar external conditions, a small and a large quantity of mass will do similar amounts of work upon their surrounding, relative to their mass. On this requirement of scale independence the entire theory of thermodynamics is based. Thus the thermodynamic system is a *source of forces*. The divergence of the force field exerted by the system (and thus also the divergence of the force field acting upon the system) is proportional to mass, hence the RHS is a linear function of V; thus div $\mathbf{f}$ is a constant, the charge density κ/V, which describes the state in which the system is. Two conclusions are here of interest:

(1) At given external conditions, div $\mathbf{f}$ is insensitive to scale. If the scale of consideration is varied which is measured in V, and since the relation of $V \propto r^3$ to $A \propto r^2$ is not linear, the relation of A to $|\mathbf{f}|$ cannot be constant; $|\mathbf{f}|$ must necessarily be a linear function of scale, $|\mathbf{f}| \propto r$. div f is the trace of the tensor $\mathbf{F}$ defined below. Both from eqn.1 and eqn.5 it follows that

$$\frac{|\mathbf{f}|}{|\mathbf{r}|} = \operatorname{div} \mathbf{f} = const \tag{2}$$

at constant external conditions, where **r** is the radius of the system, and *r* is a measure of the scale considered.[9, 11]

(2) At a given scale, the ratio *A*/*V* is a function of shape. All terms in eqn.1 RHS are insensitive to shape. Thus if the shape is thought to be changed at constant conditions, the only variable on the LHS to compensate for the change of *A* at constant *V* would be |**f**|. It is easier to think of |**f**| as to be controlled by the external conditions, though; the consequence is that the shape of the system is then fixed. It can be chosen in accordance with other constraints. Thus it follows from eqn.1 that volume, surface area, and magnitude of forces are not independent at a given state.

These conclusions are not changed by further developments of the divergence concept that can only be elaborated below, after explaining some context. Eqn.2 is in agreement with the properties of a thermodynamic continuum, with the spatial properties of a thermodynamic system that interacts with its surrounding, and with the fact that the system represents a potential of distributed matter (Ref.7, p.156). A limit operation with respect to *V* would not change the relation in eqn.2, but it would vanish identically if *r* reaches 0. This is in accordance with potential theory (Ref.7, p.147), and a refutation of the Cauchy lemma $-\mathbf{f}_x = \mathbf{f}_{-x}$ for which to be valid **f** must reach a finite value as *V* and *r* vanish.[2, 14, 15]

5. The New Approach

The fairly straightforward methods of field theories have turned out to be too simplistic to describe the deformation of a solid. The reason is that heat flow, magnetic, gravitational and electromagnetic forces may be visualized as free flow of infinitesimal quantities without internal coherence which merely follow a gradient. Solids are internally bonded; free motions are impossible. None of the theories for other natural phenomena described by vector fields had to accommodate the physical concept of the lever. Whereas tangential heat flow or tangential chemical gradients are without effect on a system they pass, mechanical shear forces do work on the system, and the work done by shear forces with opposite sense of rotation does not cancel, but it adds.

Consider Newton's body of solid with finite size and shape dropped into a fluid. The currents in the fluid represent the external boundary conditions, the shape of the body represents the material properties, the body itself represents a thermodynamic system. Let the properties of the fluid approach the properties of the solid; the system is still there, defined by its mass, only its interface with the 'fluid' is virtual, but external boundary conditions, material properties, and the equilibrium conditions are unchanged. The theory is scale-independent as in thermodynamics, so the 'body' is merely a helping concept. A system subjected to shortening in x_3 will expand in x_1 by itself if it is allowed to; in addition, the boundary conditions may actively stretch the system in x_1; both effects need to be considered separately. Two independent force fields are involved, and their interaction is not merely a superposition: the field that is derived is the result of (1) the vector field representing the external forces doing work on the system, (2) the vector field representing the material properties, and (3) the condition that system and surrounding are

solidly bonded such that disequilibrium cannot occur even if the first two vector fields have initially incompatible properties. The theory is free of proportionality constants, with the exception of z in eqn.13; the material is assumed to be isotropic. The condition of zero volume change for an isotropic material subjected to plane pure shear in the end is a prediction, but not a boundary condition.

5.1. Definition of the system

A thermodynamic system is defined by a chosen amount of mass. Its location in space is given by its center of mass Q in terms of external coordinates X_i. The surface points P of the system are given in the internal coordinates x_i whose origin coincides with the center of mass of the chosen system. The physical conditions at the points P in x_i are functions of Q(X_i) in the sense of the definition of a vector field, $\mathbf{T}(Q)\mathbf{x} = \mathbf{v}$, where $\mathbf{T}$ is a tensor as a function of location Q(X_i), $\mathbf{x}$ is the location vector of a nearby point P(x_i) relative to Q, and $\mathbf{v}$ is a vector located at P as a function of $\mathbf{T}$ and $\mathbf{x}$.

For a given vector function $\mathbf{x}$ the points P form a surface. The correlation between a surface point P and a particular direction vector in x_i is unique. Another direction vector passing through P can only be part of a different system with its own origin and coordinate set, and different boundary conditions may apply to it if the gradients in X_i are non-zero. It is therefore not of interest at this point in the discussion.

5.2. Derivation of the external and material force fields

The definition of a tensor is the derivative of a vector field with respect to the coordinates, or the second derivative of a scalar field with respect to the coordinates (Ref.16, p.57). Energy or a potential are such scalars. Let the external energy be U_{ext} and the material internal energy be E, so

$$\frac{\partial U_{\text{ext}}}{\partial x_i} = f_i \qquad\qquad \frac{\partial E}{\partial x_i} = m_i \tag{3}$$

$$\frac{\partial^2 U}{\partial x_i \partial x_j} = \frac{\partial f_i}{\partial x_j} = \mathbf{F} \qquad\qquad \frac{\partial^2 E}{\partial x_i \partial x_j} = \frac{\partial m_i}{\partial x_j} = \mathbf{M} \tag{4}$$

$$\sum_i \int_{r_j} \frac{\partial f_i}{\partial x_j} dx_j = \mathbf{Fr} = \mathbf{f} \qquad\qquad \sum_i \int_{r_j} \frac{\partial m_i}{\partial x_j} dx_j = \mathbf{Mr} = \mathbf{m} \tag{5}$$

where $\mathbf{r}$ is the radius, or the position vector of a point P on the surface of the system, $\mathbf{f}$ is the external force field; $\mathbf{m}$ is the material force field, or just the material field; and $\mathbf{F}$ and $\mathbf{M}$ are the tensors controlling the properties of the vector fields. $\mathbf{F}$ represents the external boundary conditions, and $\mathbf{M}$ represents the properties of the material which may be understood as a set of internal boundary conditions.

Since externally unbalanced forces cannot cause a deformation, they can be ignored. External equilibrium (Newton's equilibrium condition) is therefore a precondition. Also ignored are body forces as they interact with the inertial mass, but not

with the thermodynamic mass. The internal (thermodynamic) equilibrium condition is then given by

$$\mathbf{f} + \mathbf{m} = 0 \tag{6}$$

at any point P on the surface of the system, or, if **f** and **m** are understood as functions of directions θ,

$$\oint \mathbf{f}\, d\theta = -\oint \mathbf{m}\, d\theta \tag{7}$$

as a sum around the system in 2D.

The external torque is balanced by definition since the interface between system and surrounding is bonded; the disequilibrium case cannot occur in an elastic medium as long as no bonds are broken. The condition

$$\int \mathbf{f} \times \mathbf{r}\, d\theta = 0 \tag{8}$$

is an equilibrium condition with surprising freedom because *f* and *r* may vary in a reciprocal way without changing the result. If $\partial r/\partial\theta = 0$, eqn.8 is a statement of orthogonality, describing the properties of the external boundary conditions. The torque of the external forces may be balanced with additional help from surface bonding forces $\mathbf{m}_s$. The complete condition for the balance of torque is

$$\int \left(\mathbf{f} \times \mathbf{r} - \mathbf{m}_s \times \mathbf{r}\right) d\theta = 0 \tag{9}$$

where $\mathbf{m}_s \perp \mathbf{r}$, their magnitude is invariant,

$$\frac{\partial |\mathbf{m}_s|}{\partial \theta} = 0\,, \tag{10}$$

and $\mathbf{m}_s \times \mathbf{r}$ has the same sign at all surface points P. Surface bonding forces are neither external forces nor material forces; they are constraint forces which do not do work on either system or surrounding, but they make the interaction of system and surrounding possible. Their existence is concluded from the precondition that equilibrium must exist; they balance the torque of **f** if necessary. The matter is only touched here, and explained in greater detail in the chapter on simple shear.

Eqn.6 and eqn.7 differ from the Euler-Cauchy approach in the clear distinction of *system and surrounding*, of material force and external force, i.e. in the recognition of a material force in its own right. It is exerted by the system upon the surrounding due to a change of state in the system resulting from the action of external forces. The system thus represents a potential. Equilibrium between system and surrounding implies that for isotropic conditions,

$$\operatorname{div} \mathbf{f} + \operatorname{div} \mathbf{m} = 0\,; \tag{11}$$

eqn.11 therefore consists of two Poisson equations. Note that it is impossible to define a shear strength. Whether **f** at a particular point P ≠ Q is a normal force or a shear force is determined by its angular relation to the position vector **r**. However, since the material vectors **m** are always parallel radius vectors, a cross product of **r** with **m** is meaningless.

The loaded state has a scalar property, the work done, and a vector field property, the force vector field $\mathbf{f}_{\text{total}}$ resulting from the interaction of the two independent force fields **f** and **m**, the exterior and the material force field, and their respective boundary conditions in the state of equilibrium, plus the surface bonding forces if necessary,

$$\mathbf{f}_{\text{total}} = f(\mathbf{f}, \mathbf{m}, \mathbf{m}_s)\,. \tag{12}$$

$\mathbf{f}_{total}$ is not merely the sum of **f**, **m**, and $\mathbf{m}_s$.

5.3. Boyle's law for solids: the equation of state

The ideal gas law, $PV = nRT$, disregards the atomic structure of matter and considers bulk behavior only. Boyle's law can be understood as a material law for ideal gases since it predicts a particular behavior of the gas upon a change of external conditions. It relates the internal energy of a system, its mass and volume to one another and thus fully describes the energetic state in which the system is. In principle, such a description of state must also exist for solids. It must therefore be possible to define an ideal solid.

No interaction of molecules is implied in the concept of the ideal gas. If they exist, an internal pressure P_{int} is observed, such as in fluids or solids. The internal pressure of a solid is defined as the pressure that would be observed within a volume representing the molar volume of solid if it were filled with one mole of ideal gas. That pressure is balanced internally, so the internal pressure is a measure of the bonding strength of the substance. Because it is balanced, a solid is said to be in equilibrium with itself. Work must be done on the system to change this ideal density either way.

A solid in a vacuum has its ideal molar volume. Since it is able to maintain its internal pressure in a vacuum, it is necessary to scale an external pressure increase to the P_{int} with which it will interact. A generalized Boyle's law must still observe the constraints that the graph must not cross the coordinates in a P/V-diagram. This can only be done through an exponent,

$$P^k V = z \tag{13}$$

where

$$k = \frac{\ln V_{mol}^{solid}}{\ln V_{mol}^{ideal\ gas}} \ . \tag{14}$$

The law predicts that all solids have the same compressibility dV/dP if the external loading pressure is expressed in multiples of the natural internal pressure of the substance, which is easily calculated from its molar volume. $z = f(P)$ is a number characteristic for a particular state, the function is not known. The quantum-mechanic problem as to how the volume of a solid comes about, is unsolved. It is therefore not possible to predict z, but it can be modelled through the Birch-Murnaghan equation. The latter is phenomenological, but it is successfully applied in studies of material behavior under high pressure, e.g., the prediction of the elastic properties of the Earth´s core.[17] The concept is believed to be largely identical to Grüneisen's theory which is also phenomenological.[18]

Bridgman compressed the alkali metals to 100 kb.[19] It is found that they all follow the same pattern to a first approximation if the externally applied load is normalized with respect to the internal pressure of the solid (Fig.1). Thus it seems justified to use the internal pressure as a standard for the behavior of a particular material. Since eqn.13 is isotropic, k is independent of directions and only important for the modeling of real materials. For the purposes of this paper k is assumed to be unity so that $z = const$. In that

sense, the thermodynamic properties of the ideal solid are those of an ideal gas, and Boyle's law applies.

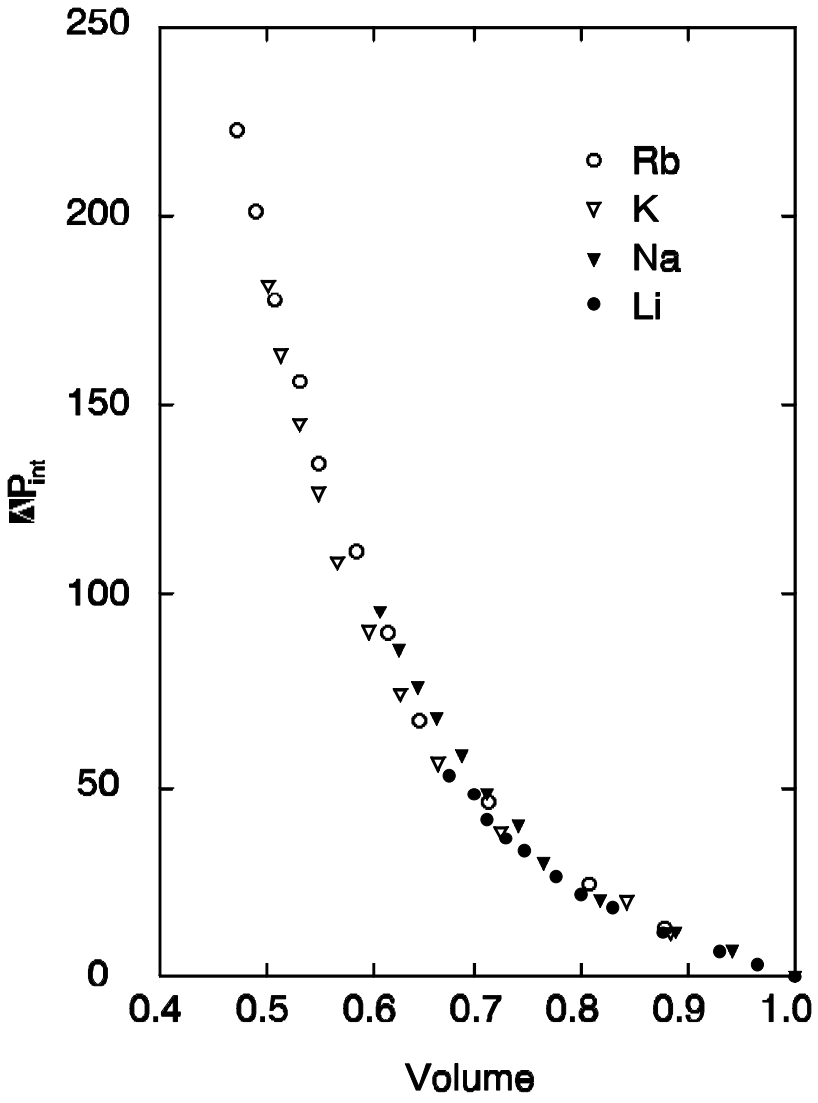

Fig.1 Compressibility data for the alkali elements. Externally applied load given in multiples of internal pressure. Data adapted from Ref.19:180).

5.4. Boyle´s law for anisotropic states

The most basic material law in thermodynamics is the Boyle-Mariotte law,

$$PV = const \tag{15}$$

The LHS is only the most common interpretation of the product. It may also be inter-

preted as a vector form of Boyle's law,

$$\mathbf{p} * \mathbf{f} = const \tag{16}$$

where **r** is the position vector of a point P on the surface of the system relative to its center of mass Q. The asterisk indicates that this product involving two vectors is yet undefined. Note that the unit (Joule) is unchanged. Boyle's law is generally given in scalars. It is therefore interpreted to be isotropic by nature.

Work in anisotropic states is not a straightforward subject. For instance, consider a rod subjected to a tensional force parallel to the horizontal direction. The effect, an elongation parallel to x_1 and a shortening parallel to x_2, is known as necking; the ratio of necking to stretching is Poisson´s ratio ν. In the present context, however, it is interesting to note that due to a force parallel to x_1, a displacement was observed, and thus work was done, parallel to x_2. Since work is a scalar, the isotropic properties of Boyle's law are here used as a boundary condition: it is assumed that the star product $\mathbf{r}*\mathbf{f}$ interpreted as

$$\mathbf{p} * \mathbf{f} = \sqrt{\left|\mathbf{p}\times\mathbf{f}\right|^2 + \left|\mathbf{p}\cdot\mathbf{f}\right|^2} = \left|\mathbf{p}\right|\left|\mathbf{f}\right| = const \tag{17}$$

must be invariant with respect to direction. $\mathbf{r}*\mathbf{f}$ gives the work done by an external force **f**, both normal and shear component, at the point P with position vector **r** on the surface of a thermodynamic system. Eqn.17 is known to be an identity. If **r** is a unit vector, $\mathbf{r}*\mathbf{f} = |\mathbf{f}|$; however, the ratio of $|\mathbf{r}|$ to $|\mathbf{f}|$ may now be a function of direction while eqn.17 is still observed if $|\mathbf{f}|$ and $|\mathbf{r}|$ maintain a reciprocal relation.

(This author is not aware of the use of an earlier equation of state in vector form in continuum mechanics, though in thermodynamics there is one, by Clausius and Grüneisen, [Ref.11, eqn.4; Ref.18, 20]. The first term in Ref.11, eqn.4a LHS is ignored here since heat can acquire importance only at temperatures above the diffusion limit, resulting in time-dependent material behavior which is not considered here.)

The only way to prevent the rod from necking would be to apply forces all over the length of the rod that would keep the surface points in place. That is, the work done during the stretch parallel to x_1 is work done by the surrounding on the system, whereas parallel to x_2 the system is doing work on the surrounding. It would require more work by the surrounding to reverse the work done by the system, and the energetic state of the system would be higher than if necking were allowed to occur. Thus the necking (or bulging, in compression) is an effect of the least work principle: some of the energy fluxes entering the system at some point are redirected inside, and returned to the surrounding at another point where the boundary conditions permit it. The stored energy is thus kept at a minimum, and the most work would be required for an isotropic compression. (The argument illustrates that energetically, deformation is inherently a three-dimensional problem. The simplified two-dimensional approach of this paper already lacks some realism; but it is not possible to reduce deformation to a one-dimensional problem, except for isotropic contractions/expansions of isotropic materials.) Starting a loading history from some given isotropic ambient pressure, the force field $\mathbf{f}_{total}$ that is building up, can therefore be decomposed into an isotropic component, the operative field $\mathbf{f}_{op}$ that represents the change of state, i.e. the work, and a deviatoric component $\mathbf{f}_{dev}$ the energetic bulk effect of which is zero. Through $\mathbf{f}_{op}$ a reference state is established which can be used to give signs to the two directions of the deviatoric field (Fig.2).

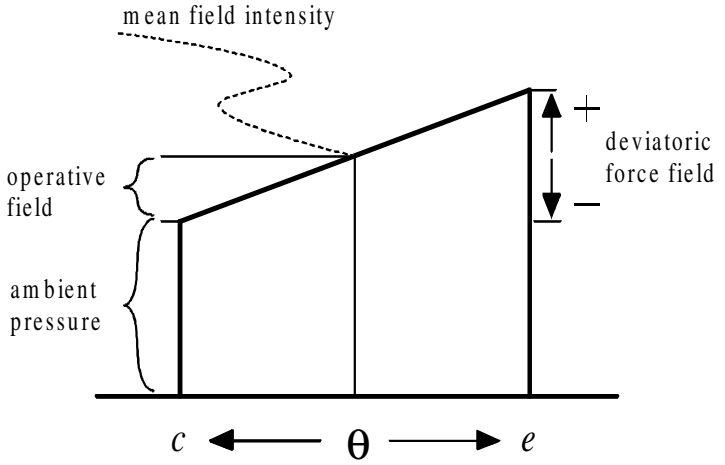

Fig.2 Relation of $\mathbf{f}_{op}$ to $\mathbf{f}_{dev}$. The vertical scale gives the magnitude, the horizontal scale gives angular directions. The left and right vertical bar indicate a contracting and an extending eigendirection (*c* and *e*) of an anisotropic force field. Figure shows relation of minimum and maximum force magnitudes to isotropic average. Shear components cannot be considered in this sketch. Ambient pressure and operative field are hydrostatic.

In contrast to gases and fluids, solids can support shear forces, and the energetic state of a system is changed by work done by shear forces and normal forces alike. A normal force will cause an expansion or a contraction of the system, depending on its sign. The sign of shear forces indicates which way the body would spin if they were unbalanced, but it gives no hints regarding volume effects. In the Euler-Cauchy theory, the matter cannot be discussed because shear forces acting on a free surface do not interact with a volume and radius in Euclidean space.

The volume effect of shear forces can be only dilational. A deviatoric force field $\mathbf{f}_{dev}$ can be partitioned into a normal component field $\mathbf{f}_n$ and a shear component field $\mathbf{f}_s$. Assume a spherical volume being subjected to the shear components $\mathbf{f}_s$ of a force field with orthogonal eigendirections, with the origin of the coordinates at the center of mass. Along the surface, all $\mathbf{f}_s$ will act on the surface points P with position vectors $\mathbf{r}$; the points P will be displaced parallel to the direction of $\mathbf{f}_s$ to the deformed position P´ with position vector $\mathbf{r}´$. Since $\mathbf{r}$ and $\mathbf{v} = \mathrm{P} \rightarrow \mathrm{P}´$ are mutually perpendicular, $|\mathbf{r}´|$ will be larger than $|\mathbf{r}|$. Therefore the work done by a shear force has a volume effect, and it is always dilational. The dilational component accumulates from zero at the contracting eigendirection towards the extending eigendirection where it reaches its maximum. This effect holds both for shear forces exerted by the surrounding on the system, and for shear forces exerted by the system on the surrounding. The combined effect of the work done by shear forces results in two additional force field components $\mathbf{m}_{s(int)}$ and $\mathbf{f}_{s(ext)}$ parallel to the extending eigendirection, such that due to the existence of shear forces a dilational (i.e. normal) effect is produced. Thus

$$\mathbf{f}_{total} = \mathbf{f}_{op} + \mathbf{f}_{dev} + \mathbf{m}_{shear} + \mathbf{f}_{shear} \tag{18}$$

where $\mathbf{f} = \mathbf{f}_{op} + \mathbf{f}_{dev}$, $\mathbf{F}_{op} = c\mathbf{I}$, and det $\mathbf{F}_{dev} = \pm 1$, and the extra terms $\mathbf{m}_{shear}$ and $\mathbf{f}_{shear}$ are not independent energetic terms, but the energetic contribution of the shear forces. An example is given below.

Work is then calculated in analogy to *PdV*-work,

$$\int f dr = c \int \frac{dr}{r} = c \ln r \tag{19}$$

The relation of material distance, i.e. the radius r_0, to a colinear force is derived through differentiation of eqn.17,

$$r_0 df + f_0 dr = 0 \tag{20}$$

If eqn.20 is divided by r_0, integrated, and divided by f_0, it follows that

$$\ln\left(\frac{r_1}{r_0}\right) = -\frac{\Delta f}{f_0} \tag{21}$$

in complete analogy to $\ln (V_1/V_0) = -\Delta P/P_0$ in isotropic thermodynamics. Eqn.21 provides the cause-effect relation, by which the displacement field $\Delta\mathbf{r} = \mathbf{s}$ is generated from the applied force field **f**.

A solid in a vacuum has its ideal volume V_0 with unit radius r_0. The internal pressure P_{int} of a solid is in the order of several kbar. In directional terms, the analogue to P_{int} is the internal force $\mathbf{m}_0$ which is a non-zero dormant force as it is internally balanced in the unloaded state. For modelling purposes it is set to unity in the following text. Above it was explained that the work done by shear forces on a volume is a dilation. Thus, be it a normal component $\mathbf{f}_n$ or a shear component $\mathbf{f}_s$, their combined effect, colinear with x_i needs to be considered. The magnitude of the externally effective force must be scaled to that of the material force $\mathbf{m}_0$, so the complete form of eqn.6 in is

$$-\Delta\mathbf{m} = \Delta\mathbf{f}_{ext} = \frac{|\Delta\mathbf{f}_{ext}|}{|\mathbf{m}_0|}\frac{\mathbf{f}_{ext}}{|\mathbf{f}_{ext}|} \tag{22}$$

where the first RHS term gives the magnitude of $\mathbf{f}_{ext}$ in multiples of the internal pressure of the material, and the second term is a unit vector with the orientation of $\mathbf{f}_{ext}$. This normalization is always implied; subsequently unit magnitude is used, and $\Delta\mathbf{f}$ is simply referred to as **f**.

If eqn.1 is called the normal divergence, the cross form of the divergence theorem (Ref.16, p.201) would be $\int \mathbf{f} \times \mathbf{n}\, dA = \int \text{curl}\, \mathbf{f}\, dV$. The equation is meaningless in the present context because it is insensitive to shear work done by fields for which curl **f** = 0, i.e. if the eigendirections of **f** are orthogonal. Since external equilibrium is always maintained due to the bonds across the surface of the thermodynamic system, a field with curl $\mathbf{f} \neq 0$ cannot rotate a system externally, but it has real, non-orthogonal eigendirections. Thus the rotation is internal, i.e. it is expressed as shear. A field with curl **f** = 0, however, does work through shear forces which are not properly represented by any expression that refers to invariants of the field property tensor. Whether internal rotation i.e. shear takes place or not, is determined not by the curl, but by the shear divergence defined as

$$\int |\mathbf{f} \times \mathbf{n}|\, dA \tag{23}$$

which is zero only if $\mathbf{F} = c\mathbf{I}$. Eqn.23 is dependent on the shape of the thermodynamic

system; as with Stokes' theorem, there is no straightforward way to transform it into a volume integral. The total divergence is then

$$\operatorname{div} * \mathbf{f} = \int \left\| \mathbf{f} \times \mathbf{n} \right| \mathbf{t} + \left(\mathbf{f} \cdot \mathbf{n} \right) \mathbf{n} \Big| \, dA \tag{24}$$

at constant V per unit mass, where $\mathbf{t} \perp \mathbf{n}$.

6. Forces and Material Reactions in Pure Shear Deformation

The condition of equilibrium for the torque is dependent on the properties of the force field and the shape of the system. The variability of the shape is constrained by the properties of the external force field, the material properties, and the condition that system and surrounding are bonded. If the effect of a progressive deformation is demonstrated in 2D, commonly a circle is transformed by a displacement field into an ellipse. The unit circle of the undeformed state as a geometric device is certainly adequate for this purpose; but the shape of the thermodynamic system (or volume element) must fulfil the equilibrium conditions. Specifically, the thermodynamic system may have an elliptical shape in one particular set of conditions, but it may be a circle in another. The two concepts – a circular pattern of points in the undeformed state vs. the mechanically active shape of the system – must not be mixed up.

Second point, strain is a function of the displacement field. If the principal axes of the strain ellipsoid do not rotate during progressive deformation they must coincide with the characteristic directions of the displacement field (and thus the force field). It can therefore be concluded that the *eigendirections* of the force field are mutually perpendicular, or that the force field, and hence the displacement field, are orthogonal. From a mathematical point of view this is a rather special case, however, and by no means a precondition. The strain tensor is thus not a helpful term to understand the physics of deformation. It is therefore necessary (a) to establish the shape of the system from the equilibrium conditions, and (b) to find the eigendirections of the force field. They are defined as the directions along which the force field **f** has no shear force components.

6.1 Shape of the volume element

Eqn.17 gives constraints for the shape of the system. The simplest shape is the sphere – it is isotropic, minimizes the A/V ratio, and for any point source at the center of mass its surface is an equipotential surface. For isotropic external conditions and an isotropic material a spherical shape for the system is the most natural choice as there are no shear forces. For other deformation types eqn.17 implies that radius and normal force along the contracting eigendirection c and those along the extending eigendirection e are identical in magnitude. The curl of the pure shear deviatoric field (Fig.3)

$$\mathbf{F}_{\text{dev}} = \begin{bmatrix} -\dfrac{\partial f_2}{\partial x_2} & 0 \\ 0 & \dfrac{\partial f_1}{\partial x_1} \end{bmatrix} \tag{25}$$

is zero; therefore the eigendirections of the resulting force field coincide with those of $\mathbf{F}_{\text{dev}}$. The conditions tr $\mathbf{T} = 0$ and det $\mathbf{T} = \pm 1$ are both conservation conditions und must hold simultaneously, hence $|F_{11}| = |F_{22}| = 1$. Since $\mathbf{F}_{\text{dev}}$ is orthogonal, there are no constraints from the equilibrium conditions on the shape of the volume element; it is therefore still spherical in shape.

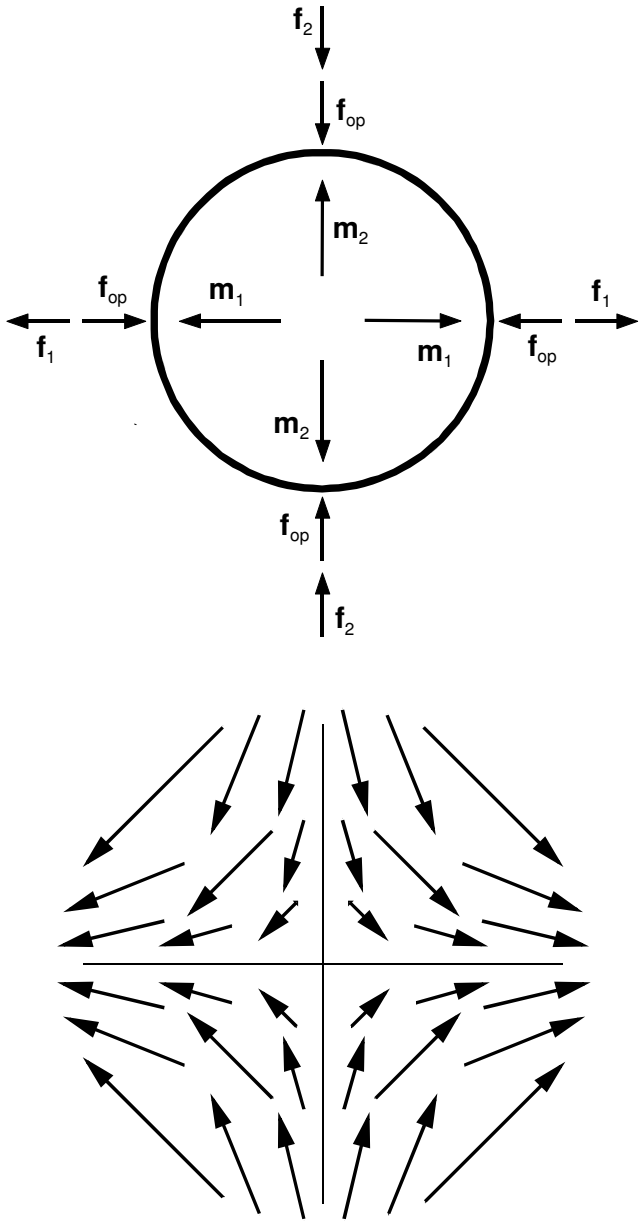

Fig.3 Pure shear deviatoric force field. Upper panel: the eigendirections of the deviatoric force field $\mathbf{f}_i$ are mutually perpendicular and parallel to the coordinates. The same figure represents the displacement field or flow field if the arrows represent displacements. $\mathbf{m}_i$: material vector, $\mathbf{f}_{op}$: hydrostatic operative pressure, $\mathbf{f}_i$: deviatoric force field. Lower panel: orthorhombic total force field, schematic.

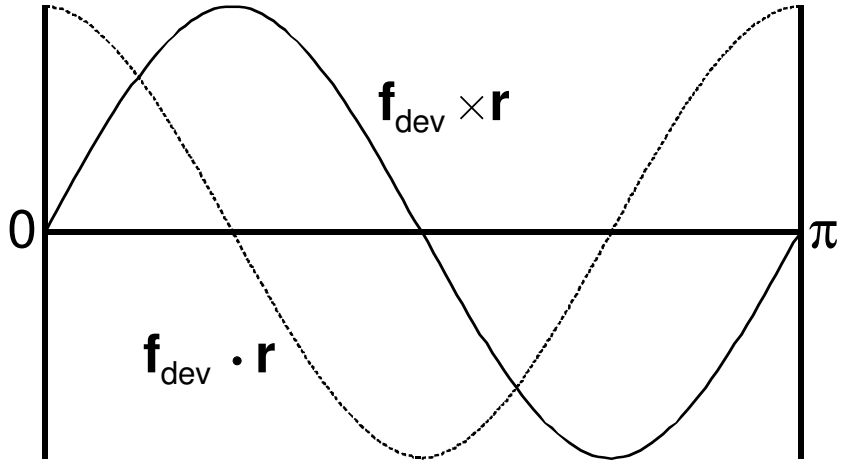

Fig.4 Force magnitude around the unit body in pure shear deformation. Horizontal axis: angular distance from one contracting eigendirection to the other. Continuous line: $\mathbf{f}_n$, broken line: $\mathbf{f}_s$. Their sum is 1 at all surface points.

The magnitudes of normal and shear deviatoric forces are shown in Fig.4. Under the given boundary conditions, all deviatoric forces on the surface have the components $\mathbf{f}$ = [cosθ -sinθ] where θ is the angle between the orientation of $\mathbf{r}$ and the x_1-coordinate. The external equilibrium condition for the torque for the entire body is then

$$\int_0^{2\pi} \mathbf{f} \times \mathbf{p}\, d\theta = 2\int_0^{2\pi} \cos\theta \sin\theta\, d\theta = 0\,, \tag{26}$$

i.e. it is balanced without the help of the surface bonding forces $\mathbf{m}_s$.

6.2 Kinematics of pure shear

$\mathbf{m}_0$ is the material force which is in equilibrium with a vacuum. For a body with unit radius in an orthorhombic deviatoric field, the components of the position vector $\mathbf{r}$ of surface point P are $[r_1\ r_2]$ = [cosθ sinθ]; the operative force vector is a normal force with components $\mathbf{f}_{op}$ proportional to [-cosθ -sinθ]; the deviatoric force $\mathbf{f}_{dev}$ is proportional to [cosθ -sinθ]; and the radius-normal unit vector $\mathbf{t}$ = [sinθ -cosθ].

External forces acting on point P are the isotropic operative force $\mathbf{f}_{op}$ and the deviatoric component $\mathbf{f}_{dev}$. $\mathbf{f}_{op}$ consists of normal components only. $\mathbf{f}_{dev}$ can be split into a normal component $\mathbf{f}_{n(dev)}$ and a tangential component $\mathbf{f}_{s(dev)}$. The sum of all normal components is

$$\Sigma\mathbf{f}_n = \mathbf{f}_{op} + (\mathbf{p} \cdot \mathbf{f}_{dev})\mathbf{p} = 1 + (\cos^2\theta - \sin^2\theta) \tag{27}$$

The respective inward-directed displacement vector $\mathbf{s}_n$ parallel to $\mathbf{r}$ is found through eqn.21.

The cross product

$$\left|\mathbf{f}_{s(dev)}\right| = 2\cos\theta\sin\theta \tag{28}$$

is equivalent to $\mathbf{f} \cdot \mathbf{t}$. A shear force has the effect that P is displaced away from the contracting eigendirection, and towards the extending eigendirection (Fig.5). The components of $\mathbf{f}_{s(dev)}$ at P evoke elastic material forces of equal magnitude and opposite sign within the system such that the torque at P is balanced. The effect of $\mathbf{f}_s$ is that P is displaced to P' (Fig.5); however, since $\mathbf{f}_s$ is perpendicular to $\mathbf{r}$, the distance r' from the origin to P' will always be larger than that from the origin to P (Fig.5). That is, a shear force will always cause a local extension proportional to its magnitude. That effect is additive from point to point. The *observed* dilation at P' is therefore the sum of all dilations from the contracting eigendirection to P,

$$\int (\mathbf{f}_{dev} \cdot \mathbf{t})\mathbf{p}\, d\theta = 2\int_0^{\alpha} \sin\theta \cos\theta \sqrt{\cos^2\theta + \sin^2\theta}\; d\theta \qquad (29)$$

where α is the angular distance measured from the contracting eigendirection c at x_2 to P. For $\alpha = {}^{\pi}/_2$, $\int \mathbf{f}\cdot\mathbf{t}\, d\theta = 1$. At the lower limit of integration there is no dilational effect, naturally; the integral reaches its highest value at the extending eigendirection e although no shear forces are observed at that point.

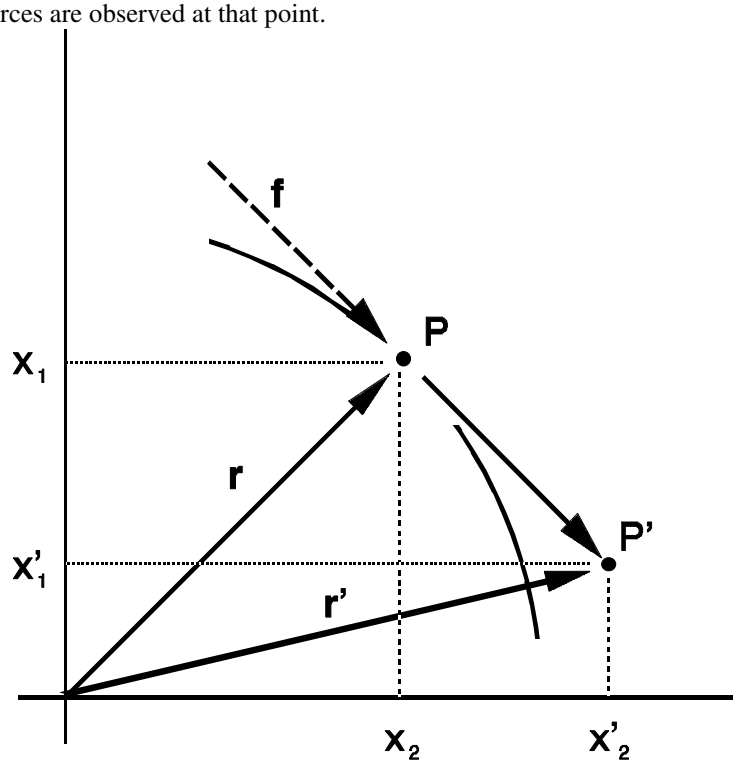

Fig.5 Dilatancy effect of a shear force component. Surface of thermodynamic system: curved line. Tangential force vector (dashed) will displace material point P towards P'; the distance from the origin is increased. Point coordinate x_1 is stretched to x_1' by horizontal component of $\mathbf{f}$, x_2 is shortened to x_2' by vertical component of $\mathbf{f}$. X_i: reference frame parallel to eigendirections.

In a continuum, the result of eqn.29 counts *twice*. This is explained through a thought experiment. Step 1: assume a body loaded hydrostatically so that the operative force field

(the change of the energetic state of the system) has magnitude -1, and the deviatoric field has magnitude zero. Along x_1 and x_2 the radius is contracted. Step 2: the boundary conditions are relaxed along x_1 only; consider the surrounding as immobile. In the attempt to reduce the stored energy, the material expands by itself parallel to x_1 whereas nothing changes along x_2. The operative field magnitude is reduced to -½, and a deviatoric field of magnitude ± ½ develops. Since the expansion is not isotropic, the body will exert shear forces at the surrounding; in the first quadrant (to the right of the contracting eigen-direction and above the extending eigendirection) it will result in a sinistral couple at the system-surrounding interface, and in a dextral couple in the second quadrant (counting clockwise). Therefore, work is done *by the system* on the surrounding, thereby reducing the energetic state of the system from -1 to -½, until the system has reached its energetic minimum state. Note, however, that the sign of the couples is opposite to what should be expected from a proper continuum pure shear case. Step 3: but if the surrounding deforms with the system, it will first expand with the system in x_1, and then exert additional shear forces on the system, causing a dextral couple in the first quadrant and a sinistral couple in the second, resulting in a further expansion parallel to x_2. This shear work is work done *by the surrounding*, and will cause an increase of the energetic state from -½ to -1. Therefore one part of the expansion is supplied by the shear effect of the material ($\mathbf{m}_{shear}$ cf. eqn.18), one part by the shear effect of the external force field ($\mathbf{f}_{shear}$ cf. eqn.18), and both are proportional to the magnitude of the deviatoric field. The result is that a dilational force of twice the magnitude of the integrated external shear forces acts upon the surface point on the extending eigendirection which will therefore be shifted away from the center of the system.

Note that the surrounding can cause shortening work on the system along x_2 whether the interface is bonded or not, whereas the surrounding can cause an extension of the system along x_1 only if the system-surrounding interface is bonded. Hence there are surface-bonding constraint forces $\mathbf{m}_s$ involved which do not do work by themselves, but without them the surrounding could not do extensional work on the system. If the interface were not bonded the extrusion of the system by itself due to $\mathbf{m}_{s(int)}$ (step 2) would still occur, but not the second component due to $\mathbf{f}_{s(ext)}$ (step 3) where the surrounding is actively pulling. In a perfect continuum with no solid-vacuum interfaces or bonding discontinuities (e.g. joints, lattice defects) nearby, both parts are observed. $\mathbf{f}_{s(ext)}$ becomes a variable in the transition from continuum mechanics to discrete mechanics and reaches zero at discontinuous surfaces, e.g. between a solid and air. An illustrated example is given at the end of this paper.

6.3 Volume effect of deviatoric loading

A numerical example, using eqn.21 (inward-directed work is positive): $r_0 = 1$, $f_0 = 1$, and volume $V_0/\pi = 1$. After loading to operative field magnitude 1/5, the magnitudes along x_2 are $\Delta f = f_{op} + f_{n(dev)} = 2/5$, $r_2 = 0.670$, and along x_1 they are $f_{op} + f_{n(dev)} = 1/5 - 1/5 = 0$, $r_1 = 1.000$; but $f_{s(int)} + f_{s(ext)} = -2/5$, so $r_1 = 1.492$. The volume of the resulting ellipse is $V/\pi = r_1 r_2 = 1$, i.e. area is preserved if compared with the unloaded state (Fig.6).

An important point is to be learned from this example. If the body had been subjected to a hydrostatic field whose change of the energetic state is identical in magnitude to that of the pure shear example, it would have undergone a contraction to r = 0.819, V/π = 0.670. This isotropic change of state is the thermodynamic ideal change of state because it requires maximum work and is characterized by the highest boundary constraints. Dilation always occurs as a function of shear forces $\mathbf{f}_s$ acting on the system if $\mathbf{F}_{dev} \neq 0$. It appears that *with respect to a hydrostatically loaded body at some given state, every anisotropically loaded body with identical energetic state is constitutionally expanded*. Dilatancy has been observed long ago, but Reynolds´s explanation is based on the assumption that the structure of matter is granular.[21, 22] The prediction here is the result of a continuum theory.

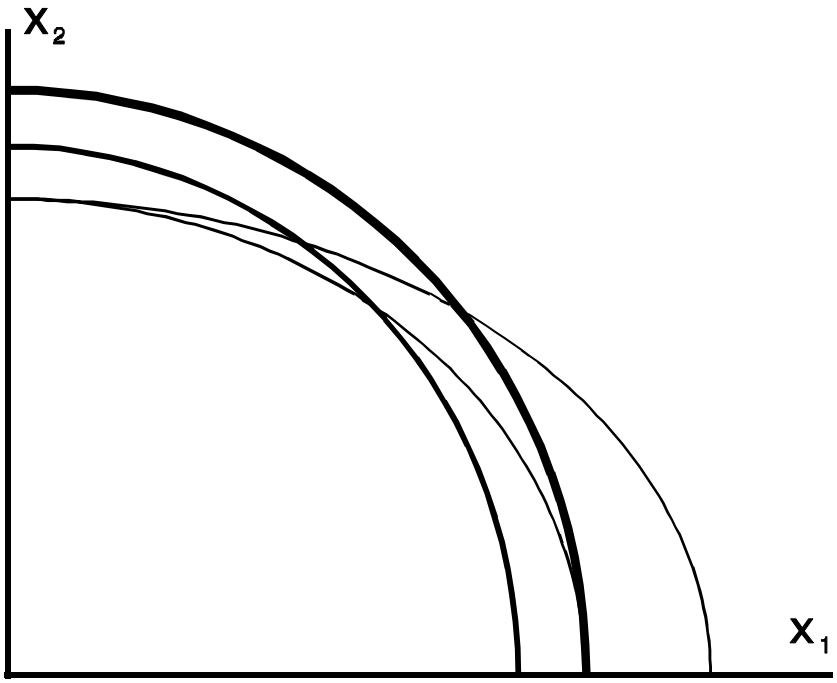

Fig.6 The making of an ellipse. Outer, heavy circle: surface of unit body before loading. Inner, light circle: unit body after hydrostatic loading due to operative field; area decreases. Inner elliptical outline: change of shape of loaded body due to normal deviatoric component only; area stays constant. Outer elliptical outline: finite strain ellipse after considering shear work. Area between elliptical outlines: area increase due to dilatancy effect. For pure shear area loss due to operative field and area gain due to shear dilatancy balance. X_i: external coordinates parallel to the eigendirections.

For the pure shear example chosen here the calculated dilation exactly balances the volume loss caused by the application of the operative field, that is, the resulting deformation is isochoric. This prediction compares well with observations in real materials in the sense that pure shear deformation is known to occur at constant volume;

the dilation with respect to the hydrostatic loaded state is not obvious. In contrast to the Euler-Cauchy approach that used volume invariance as a precondition, it is delivered as a prediction by the approach presented in this paper.

Since solids have a natural ideal density, their capacity to expand is limited. During hydrostatic compressional loading, boundary conditions do not permit a behavior that would be countereffective; however, solids cannot be expanded, and an artificial material underpressure in the solid cannot be maintained because heterogeneous behavior (i.e. cracking) is a viable alternative for the solid to maintain its equilibrium internal pressure.

7. Properties of Simple Shear

7.1 The eigendirections

The position O of the body center in space is given in coordinates X_i. A second coordinate set x_i is fixed to the body, its surface points are given relative to O in the latter system.

Simple shear is commonly illustrated by laterally pushing a deck of cards on a desk. It must be noted that the boundary conditions of this experiment deviate considerably from the conditions of an orthorhombic field as required by the Cauchy stress: (*a*) the cards are stiff in their long extensions; (*b*) the experiment does not work if the cards are wet or the stack is too high, so the coherence between the cards must be negligible; (*c*) the pushing must be done parallel to the cards and the desk, not oblique, and the pushing is gradually increased upwards. Condition (*a*+*b*) means that the material is highly anisotropic, and the assemblage of cards is not coherent; in a general theory these conditions must be dropped in favor of initially isotropic material properties (considered to be the simplest case) and material coherence. Condition (*b*) indicates that no external forces act perpendicular to the desk, not even those of the confining pressure. Condition (*c*) suggests that perpendicular to the desk there is a gradient of forces which themselves are oriented parallel to the desk. For a dextral shear the deviatoric external force field therefore has the form $\mathbf{F}_{\text{ext}}\mathbf{r} = \mathbf{f}_{\text{ext}}$ where

$$\mathbf{F}_{\text{ext}} = \begin{bmatrix} 0 & \dfrac{\partial f_1}{\partial x_2} \\ 0 & 0 \end{bmatrix} \tag{30}$$

(Fig.7a). The characteristic equation of such a field is degenerated; the eigendirections *c* and *e* coincide and are parallel to x_1. Since the eigendirection is real, there is no external rotation. The field is most unlikely to be of physical relevance by itself, at least not for a reversible process. The condition $\det \mathbf{T} = \pm 1$ is a conservation condition (the Jacobian) in a mapping; the condition $\det \mathbf{T} = 0$ is a strong indication that any kinematic concepts based on this condition (e.g., “ideal” simple shear, exemplified by the deck-of-cards model) are physically unrealistic.

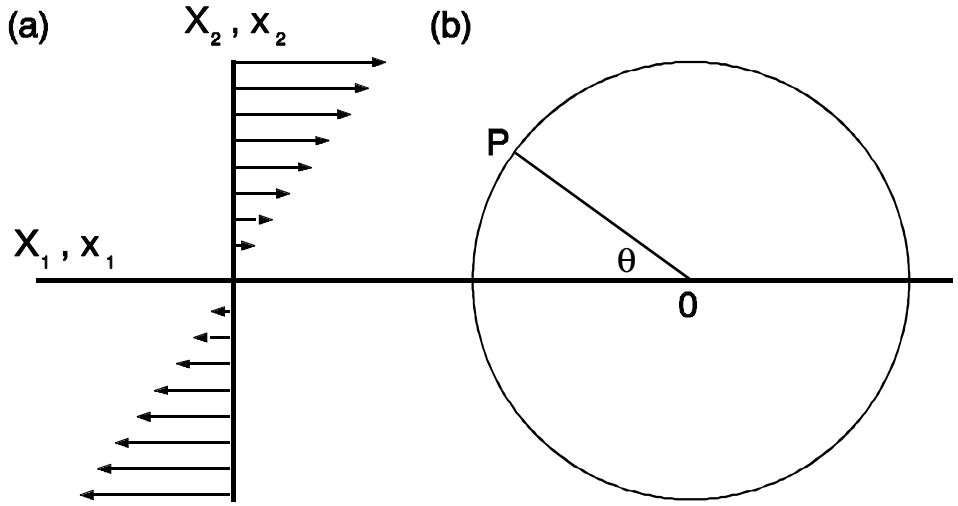

Fig.7 Simple shear external force field with unit body subjected to it. The force field only consists of forces parallel to X_1. The unit body is fixed in space and cannot rotate. P: point of action of a force vector, O: origin, θ: angle enclosed by position vector of P and x_1.

This field interacts with a unit body (the thermodynamic system) possessing isotropic material properties (Fig.7b). Thus, in a continuum an infinite number of force vectors will act at an infinite number of points of action along the surface of the system. Therefore it is necessary to find the average point of action of the average force vector $\mathbf{f}_{av}$ on the body. From the statement of the problem (Fig.7), $f \propto \sin\theta$ where θ is the angle enclosed by $\mathbf{r}$ and the reference line x_1. The average for one quadrant is found through

$$\frac{\int_0^{\frac{\pi}{2}} \sin\theta \, d\theta}{\frac{\pi}{2}} = \frac{2}{\pi}. \tag{31}$$

The average force is a vector of the form $\mathbf{f}_{av} = [2/\pi\ 0]$, and the position vector of its point of action P_κ encloses with x_1 the angle $\kappa = \pm 39.54°$ (Fig.8). If the body is fixed in space and subjected to a force field as in eqn.30, the normal force component has the form

$$\mathbf{f}_n = (\mathbf{f}\cdot\mathbf{n})\mathbf{n} = \cos\theta\ \sin\theta\,, \tag{32}$$

and the shear force component is given by

$$\mathbf{f}_s = (\mathbf{f}\cdot\mathbf{t})\mathbf{t} = \sin^2\theta\,. \tag{33}$$

At P_κ the latter is therefore

$$\mathbf{f}_{s(\kappa)} = \left(\frac{2}{\pi}\right)^2 = 0.405\,. \tag{34}$$

If the body is allowed to react to the applied force field, $\mathbf{f}_{s(\kappa)}$ is accommodated: since the coherence is maintained, external disequilibrium is impossible. Hence the system is not able to rotate freely, but surface bonding forces $\mathbf{m}_s$ will be activated parallel to its surface. Thus $|\mathbf{f}_{s(\kappa)}|$ is subtracted from all $|\mathbf{f}_s|$ at all points; the sign of the effective $\mathbf{f}_s$ will be

reversed in some areas. The effective shear force magnitude at any point P is therefore

$$\left|\mathbf{f}_{s(eff)}\right|_{\theta} = \mathbf{f}_{\theta} \cdot \mathbf{t}_{\theta} - \left|\mathbf{f}_{s(\kappa)}\right| , \tag{35}$$

and the total effective force at P(θ) is

$$\mathbf{f}_{eff} = \mathbf{f}_{s(eff)} + \mathbf{f}_{n} . \tag{36}$$

Initially there are two points with no radius-normal force components at $\theta = 0$ and $\theta = \pi$ (Fig.7b). Due to the subtraction of $\mathbf{f}_{s(\kappa)}$, these points move away from x_1 by $\theta = \pm \kappa$ to either side of the coordinate axis. Since only normal components act along these directions, they are interpreted as eigendirections (contracting: *c*, extending: *e*) which are not mutually perpendicular. They enclose the angles $\pi - 2\kappa = 100.92°$ and $2\kappa = 79.08°$. However, by using the unit vector **n** and $\mathbf{t} \perp \mathbf{n}$ in eqn.32 and eqn.33, a spherical shape of the system is implied because there is no difference yet between **n** and **r**. It is still not possible to balance the rotational momentum for a body with a spherical shape as $\int_{2\pi} \left| \mathbf{f}_{s(eff)} \times \mathbf{r} \right| d\theta \neq 0$. Therefore the assumption regarding the shape may be faulty. The angular relation of the eigendirections suggests that the effective force field $\mathbf{f}_{eff}$ for simple shear and the shape of the system both have elliptical properties. It is therefore necessary to calculate the shape of the ellipse which is in equilibrium with $\mathbf{f}_{eff}$ with eigendirections as indicated above, and which fulfils the requirement of eqn.17.

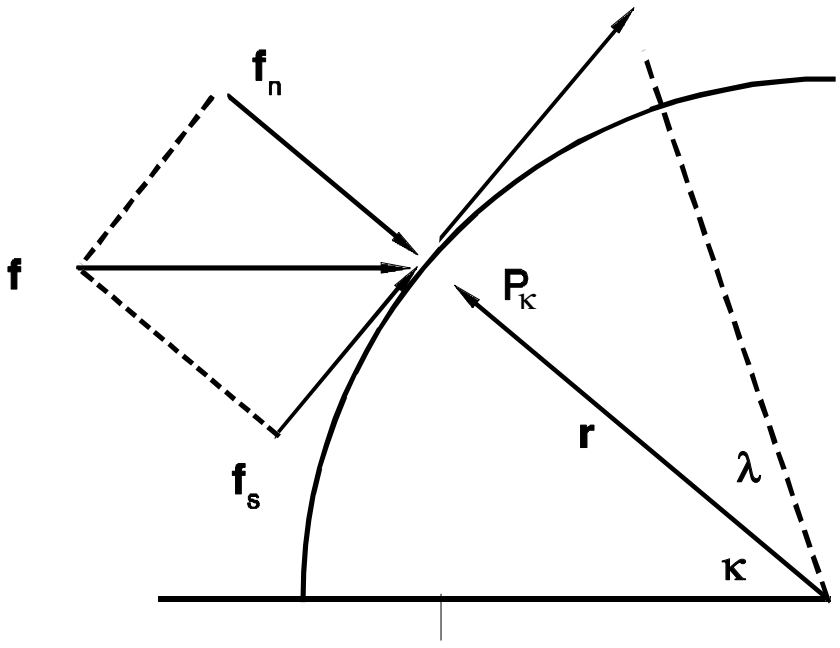

Fig.8 Forces at surface of a body in a continuum subjected to a force field as in Fig.7. Average force $\mathbf{f}_{av}$ at its point of action P_κ on surface of unit body in simple shear environment. $\mathbf{f}_{av}$ with magnitude sin κ decomposes into normal force $\mathbf{f}_n$ and shear force $\mathbf{f}_s$. The latter is accommodated by surface bonding forces. $\mathbf{f}_{s(\kappa)}$ is subtracted from shear force at all points, resulting in sinistral shear forces between P_κ and 0. λ is the angle of a coordinate transformation due to dextral shear force imbalance. The equilibrium condition $\int \mathbf{f} \times \mathbf{r}\, d\theta = 0$ holds.

7.2 Force field and shape of volume element

In the pure shear example (PS), the field property tensor (eqn.25) has the properties $\mathrm{tr}\,\mathbf{F}_{PS} = 0$ and $\det \mathbf{F}_{PS} = \pm 1$. Eqn.30 for simple shear (SS) differs in the latter point. However, the term in eqn.34 is not part of eqn.30. The field matrix for simple shear is therefore assumed to be characterized by the condition $\det \mathbf{F}_{SS} = \pm 1$ after the subtraction, indicating that all normal fluxes that are part of the deviatoric field and which enter the system, will leave it as well. Thus, the force field under the boundary conditions for elastic simple shear and the shape properties of the system are here modelled by assuming an orthogonal field of the form

$$\mathbf{F}_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{37}$$

which is in equilibrium with a system of spherical shape. The maximum shear directions should coincide with the points on the coordinates, though, so the force field is reoriented by a sinistral rotation of 45°. Both force field and radius field are then transformed by a transformation matrix $\mathbf{T}$ to acquire elliptical properties, where $\mathbf{p}$ are the position vectors of the surface points in the untransformed state:

$$\mathbf{T} = \begin{bmatrix} \cot\kappa & 0 \\ 0 & \tan\kappa \end{bmatrix}, \tag{38}$$

$$\mathbf{T}\mathbf{F}_0 = \mathbf{F}_{\mathrm{dev}} = \begin{bmatrix} 0 & \cot\kappa \\ \tan\kappa & 0 \end{bmatrix} = \begin{bmatrix} 0 & T_{11} \\ T_{22} & 0 \end{bmatrix}, \tag{39}$$

$$\mathbf{T}\mathbf{p} = \mathbf{r}_{\mathrm{ell}} = \begin{bmatrix} T_{11}\cos\theta & T_{22}\sin\theta \end{bmatrix}, \tag{40}$$

and

$$\mathbf{F}_{\mathrm{dev}}\mathbf{p} = \mathbf{f}_{\mathrm{dev}} = \begin{bmatrix} T_{11}\sin\theta & T_{22}\cos\theta \end{bmatrix}. \tag{41}$$

The eigendirections of the elliptic radius field $\mathbf{r}_{\mathrm{ell}}$ are thus mutually perpendicular, and identical to the principal axes of the resulting ellipse with area $A/\pi = T_{11}T_{22} = 1$ whereas the eigendirections of the force field – extending: $\mathbf{v}_e$, contracting: $\mathbf{v}_c$ – are non-orthogonal as desired,

$$\mathbf{v}_{e,c} = \begin{bmatrix} 1 \\ \pm\tan\kappa \end{bmatrix}. \tag{42}$$

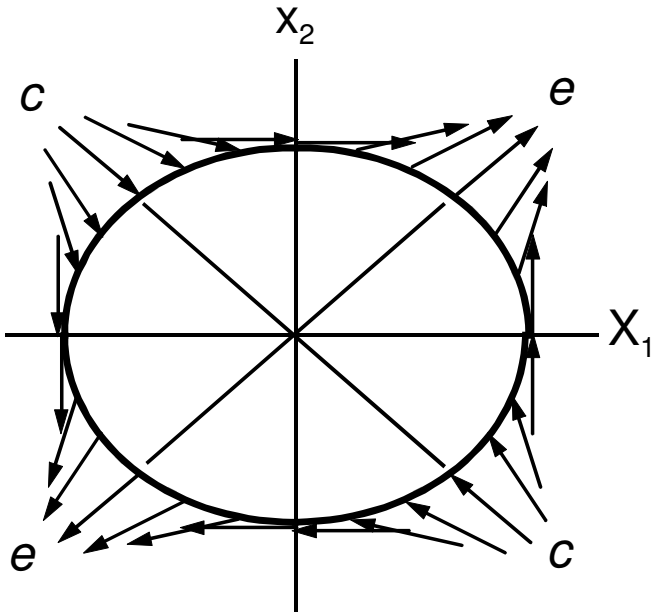

Fig.9 Thermodynamic system, or volume element, with unit mass and elliptical shape which is in equilibrium with monoclinic external force field. Acute angle between eigendirections *c* and *e* = 2κ.

7.3 Kinematics of simple shear

Conveniently, all equations regarding equilibrium conditions etc. are just transformed forms of the pure shear example, too. The cross product simplifies to

$$\oint \left| \mathbf{f}_{\text{dev}} \times \mathbf{r}_{\text{ell}} \right| d\theta = T_{11} T_{22} \oint \left(\cos^2 \theta - \sin^2 \theta \right) d\theta = 0 , \tag{43}$$

i.e. the elliptic properties of radius field and force field cancel. The sum of the normal force components is

$$\oint \mathbf{f}_{\text{dev}} \cdot \mathbf{r}_{\text{ell}} \, d\theta = \left(T_{11}^2 + T_{22}^2 \right) \oint \cos\theta \sin\theta d\theta = 0 . \tag{44}$$

Since $T_{11}^2 + T_{22}^2 > 2$, the maximum magnitude of the dot product along the eigendirections is larger than unity. This is believed to be an artefact of the elliptic shape as the radii along the eigendirections do not have unit length due to the transformation by **T**. If the force is dotted with the inverse position vector $\mathbf{r}_{\text{ell}}^{-1} = \mathbf{T}^{-1}\mathbf{r}$,

$$\oint \left| \mathbf{f}_{\text{n(dev)}} \right| d\theta = \oint \mathbf{r}_{\text{ell}}^{-1} \cdot \mathbf{f}_{\text{dev}} \, d\theta = \oint 2 \cos\theta \sin\theta d\theta = 0 \tag{45}$$

the equilibrium condition is still maintained. The elliptic properties of force field and body shape cancel, resulting in a consideration of normal deviatoric force $\mathbf{f}_{\text{(n)dev}}$ per unit radius, the maximum magnitude of which is 1. Eqn.45 gives the normalized relation of $|\mathbf{f}_{\text{n(dev)}}|$ to $|\mathbf{r}_{\text{ell}}|$; that normalization of f_{n} with respect to r is necessary (cf. eqn.22). $\mathbf{f}_{\text{op}}$ (cf. eqn.18 to eqn.21) is therefore also a unit vector. Eqn.43 and eqn.45 together observe eqn.17. Some vector magnitudes are shown in Fig.10.

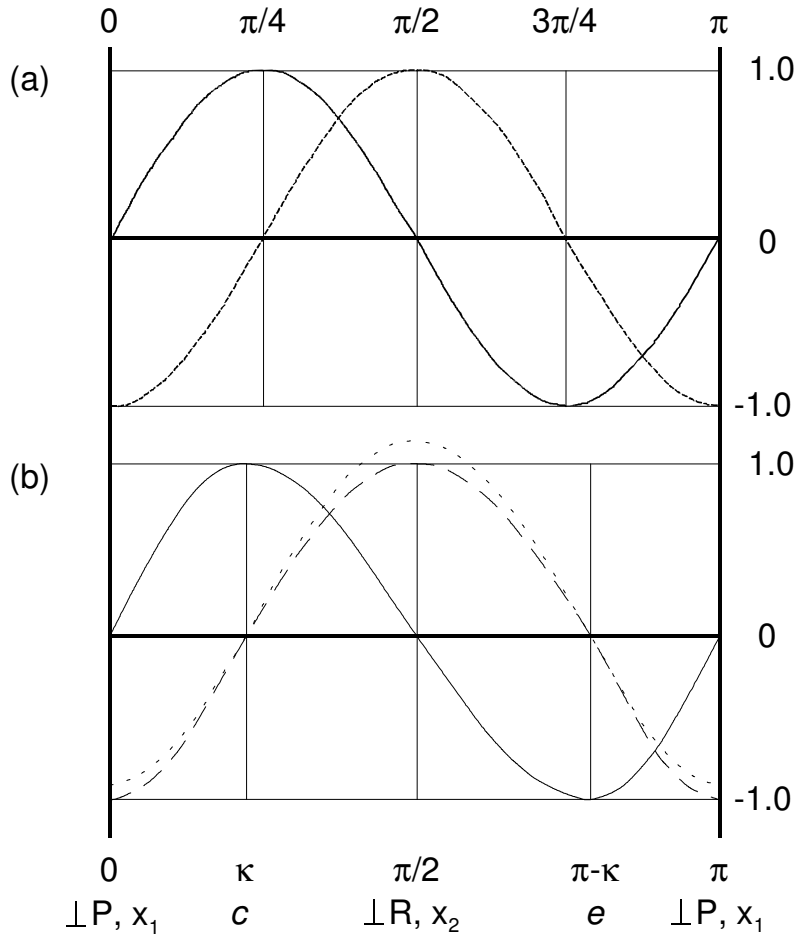

Fig.10 Vector magnitudes in simple shear. (a) in untransformed space, (b) in transformed space. Continuous line: normal component $\mathbf{f}_{n(dev)}$ (eqn.45), long dash: $|\mathbf{f}_{dev} \times \mathbf{r}_{ell}|$ (eqn.43), short dash: $\mathbf{f}_s$ (eqn.46, see text). ⊥R, ⊥P: direction perpendicular to R- and P- plane, cf. Fig.11.

If $\mathbf{t} \perp \mathbf{n}$, $\mathbf{t}$ is not a tangent vector to the ellipse, but is defined as a radius-normal unit vector, irrespective of the orientation of the elliptic surface. (This is against intuition trained on the Euler-Cauchy theory which treated stress as a force acting on a plane as a function of the orientation of the plane, but Newton's definition of the rotational momentum does not make use of planes.) The magnitude of the shear force component is given by

$$\left|\mathbf{f}_{s(dev)}\right| = \mathbf{f}_{dev} \cdot \mathbf{t} = T_{11} \sin^2 \theta - T_{22} \cos^2 \theta \qquad (46)$$

Integration for separate sectors (e.g., from the contracting eigendirection to either side towards the extending eigendirection, or from 0 to κ and from κ to π/2) shows that there is an imbalance between dextral and sinistral shear forces acting on the system. However, eqn.46 is not an equilibrium condition, the shear forces by themselves need not balance. Because forces are balanced for the ellipse (eqn.43), an imbalance in $\mathbf{f}_{s(dev)}$ cannot imply a

spin. The imbalance is therefore interpreted to indicate a permanent reorientation of the force field through a transformation of the internal coordinate axes x_i with respect to the external reference frame X_i by an angle λ such that

$$\sqrt{\left|\mathbf{f}_{s(\text{dextral})}\right| - \left|\mathbf{f}_{s(\text{sinistral})}\right|} = \tan\lambda; \quad \lambda = 28{,}83° \tag{47}$$

where the vector magnitude terms under the root stand for the integrated sums over adjacent sectors. Since the eigendirections are real, the transformation angle λ is stable. (The root is taken because all angular terms in eqn.46 are squared. The LHS in eqn.47 is interpreted as a tangent term because there is no reason why it should be restricted to values ≤ 1. As the LHS $\rightarrow \infty$, $\lambda \rightarrow 90°$, which would be the condition for external rotation. At the same instant, the characteristic equation should degenerate, whence the eigendirections become imaginary.)

Above it was explained that a shear force has the effect that P is displaced towards P', away from *c*, and towards *e*. A shear force will always cause a local extension proportional to its magnitude. That effect is additive from point to point. During a simple shear elastic deformation, the same principle holds, except that the eigendirections are no longer mutually perpendicular. However, the result is similar to that of eqn.29 (which was 1 over each quadrant), except that the surface over which the integration is performed, is larger than that of the circular volume element. The result per quadrant is therefore larger than for a circular surface by the factor $T_{11}T_{22}/2 = 1.018$. As explained in the pure shear example (following eqn.29), this result counts twice, $w_s = 2.036$.

w_s is the dilational effect of the shear forces along the radius r_e parallel to *e*. The shortening factor for the radius r_c along *c* is given by eqn.21. If $\mathbf{v}_c$ and $\mathbf{v}_e$ are the normalized eigenvectors, they can be understood as the radii of a unit circle subjected to the monoclinic field $\mathbf{Fr} = \mathbf{f}$, and the displacement field can be calculated. A numerical example, using eqn.21: $r_0 = 1$, $f_0 = 1$, and volume $V_0/\pi = 1$. After loading to operative field magnitude 1/5, the magnitudes along *c* are $\Delta f = f_{op} + f_{n(dev)} = 2/5$, $r_c = |\mathbf{v}_c| = 0.670$. Along *e* they are $f_{op} + f_{n(dev)} = 1/5 - 1/5 = 0$, $r_e = 1.000$; but $w_s = -2.036/5 = -0.407$, so $r_e = |\mathbf{v}_e| = 1.503$. If **S** is the displacement field property tensor,

$$r_c r_e = \left|\mathbf{v}_c\right|\left|\mathbf{v}_e\right| = \det \mathbf{S} = 1.0075 \tag{48}$$

indicating that in this example the volume expands by 0.75%. The expansion increases progressively, i.e. the material density decreases in elastic simple shear in comparison to the unloaded state due to excess shear work done against the internal pressure of the material. This volume increase in elastic simple shear has been observed; it is known as the dilatancy.[21, 23] From the approach presented here it becomes clear that this behavior is not unique to simple shear. It was also found in the pure shear example where it was hidden because it cancelled the contraction caused by $\mathbf{f}_{op}$, and where it cannot be expected by theoretical approaches that include the *a priori* assumption that the material is "incompressible". To this author's knowledge, the approach presented here is the first one that predicts the phenomenon of dilatancy not as a function of the material properties, but as a function of the physical set-up.

7.4 Geometric properties of simple shear deformation

The coordinates x_i are rotated with respect to X_i by λ in the sense of shear. In physical space X_i, the following picture emerges (Fig.11): the extending eigendirection *e* is at 10.71°, the contracting eigendirection *c* is at 111.63°. The bisectors of the angles enclosed by *c* and *e* are parallel to the x_i-coordinates and represent maximum shear directions. The orientation vector bisecting the large sector at 61.18° indicates a shear plane perpendicular to that orientation, the R-plane is therefore found at -28.83°; the orientation vector bisecting the small sector at -28.83° indicates the P-shear plane at 61.18° (Fig.10).

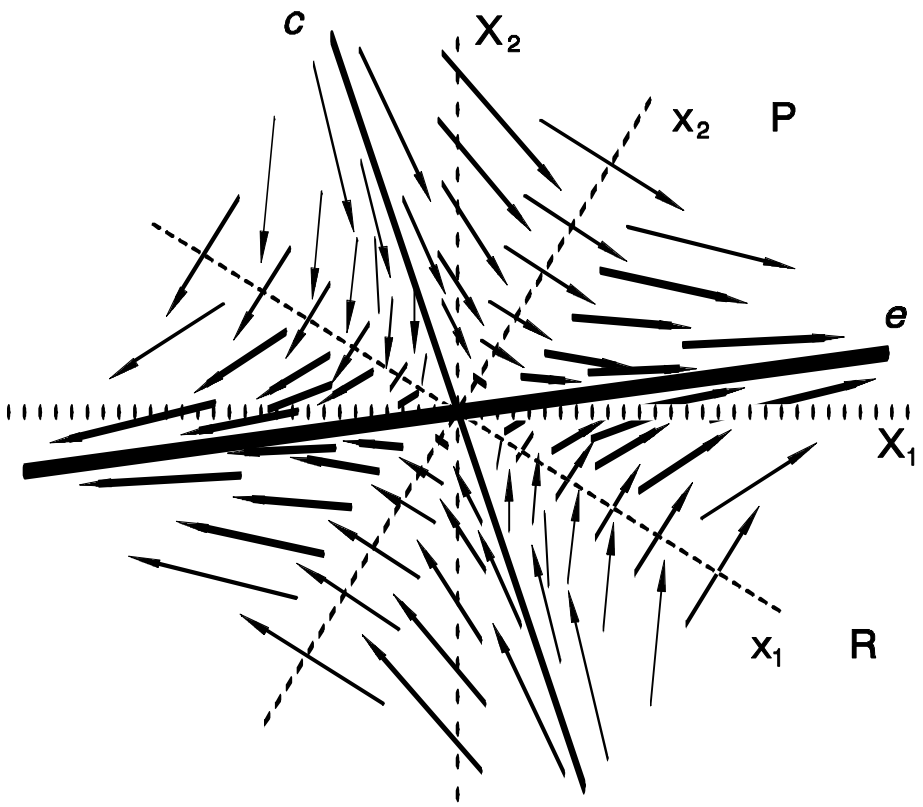

Fig.11 Dextral simple shear. Predicted flow field. Calculated geometric properties: x_i, X_i: internal and external coordinates, *c*: contracting eigendirection, *e*: extending eigendirection, R: R(iedel)-plane; P: P-plane. Despite the fact that the external force field $\mathbf{f}_{ext}$ does not have a component parallel to x_2, the effective field $\mathbf{f}_{total}$ and the displacement field both do.

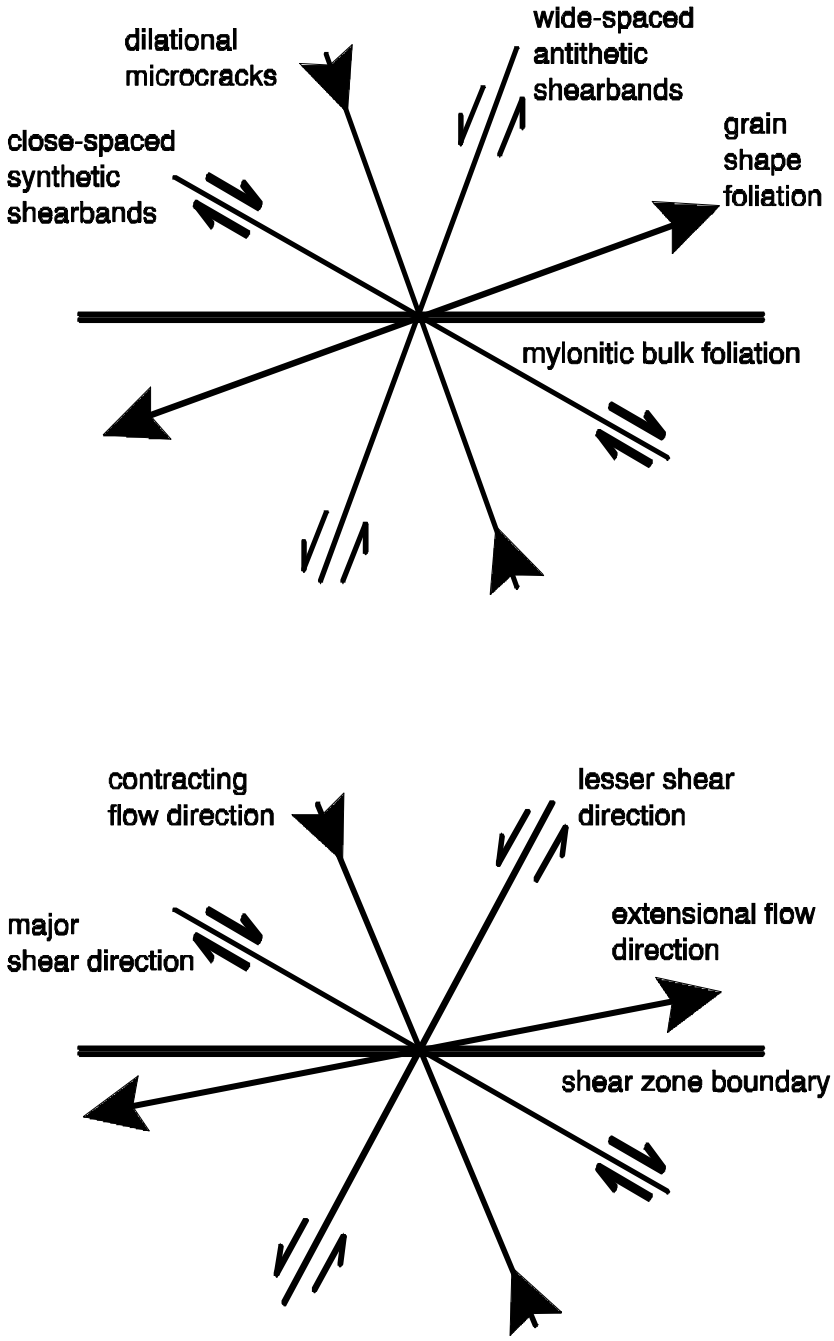

Fig.12 Geometry of simple shear. Top: Observed geometric fabric properties (after Ref.24). Bottom: calculated geometric properties (identical to Fig.11): The only major difference between observation and prediction is the orientation of the grain shape foliation of quartz (amphibolite grade metamorphic facies). However, quartz grain boundaries are highly mobile, and considered not diagnostic. The extending eigendirection is believed to correlate with the lattice preferred orientation (e.g. mica) which commonly is shallower (cf. Fig.13).

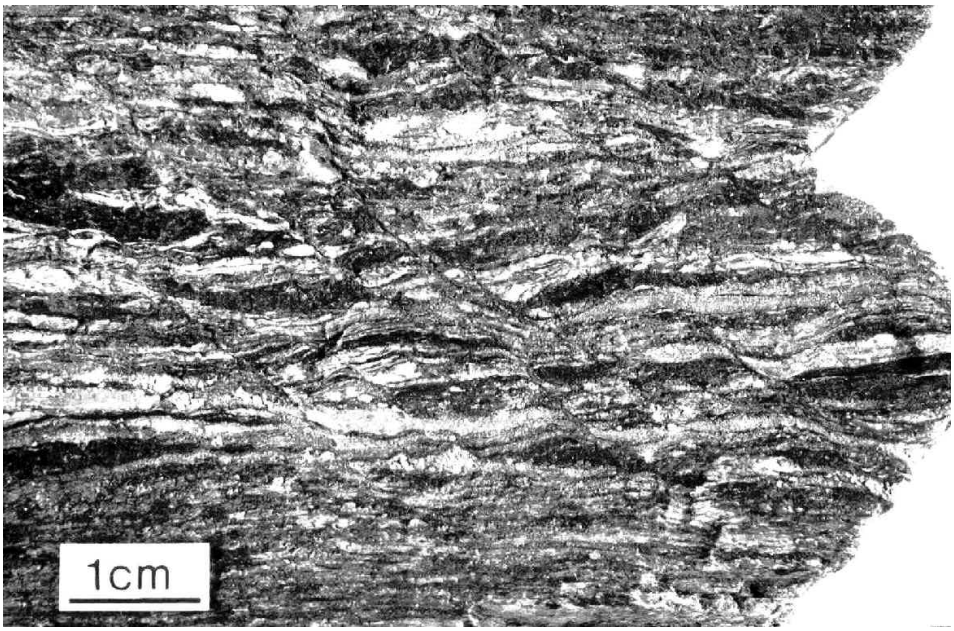

Fig.13 Dextral simple shear. Natural S-C-fabric: lower greenschist facies mylonite from the Insubric Line, Sesia Zone, Val Strona, Italy. Long edge of photograph is parallel to the bulk foliation, providing external reference frame. Shear planes moderately inclined to the right are the C-planes. Compositional layering gently inclined to the left is the S-plane. Note considerable sinistral volume rotation between C-plane discontinuites with dextral offset. Bulk sense of shear is dextral.

Fig.14 Dextral simple shear. Viscous simple shear deformation in subrecent obsidian flow, Lipari Island, Italy. Upper layer consists of black glass with vesicles, was softer, and shows drag. Lower layer consists of partly crystallized material, behaved stiffer, and reacted by fracturing. Drag in upper layer and joint orientation in lower layer indicate dextral flow.

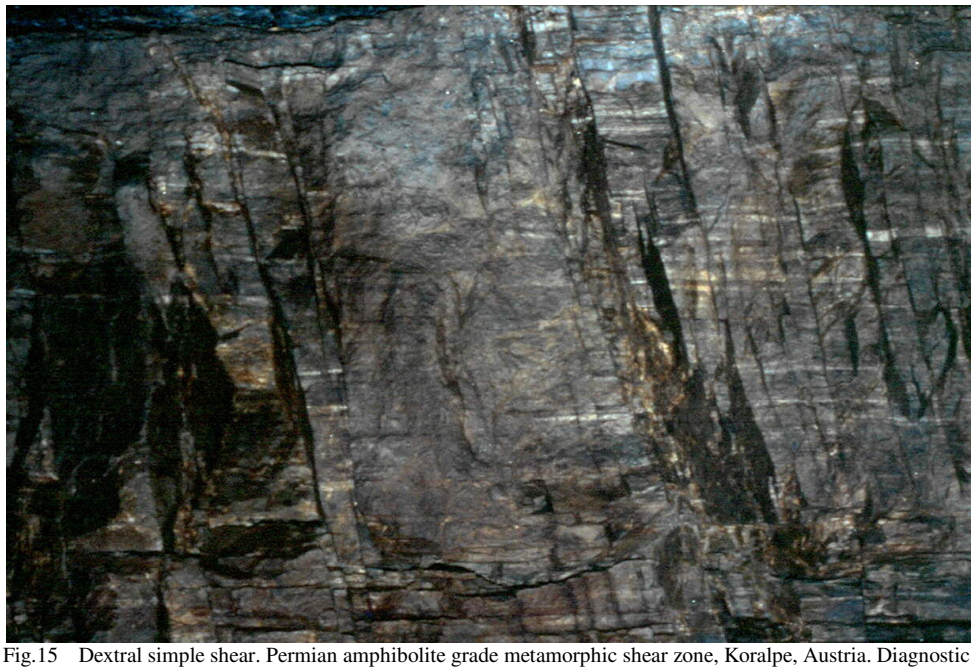

Fig.15 Dextral simple shear. Permian amphibolite grade metamorphic shear zone, Koralpe, Austria. Diagnostic joints ca.100° inclined against the sense of shear, and parallel to eigendirection *c* in Fig.11. Joints opened during late Tertiary uplift through release of residual tensions as confining pressure dropped. Vertical dimension ca.1,2m.

The topic of this paper is the force field that causes the deformation, and the displacement field. But irrespective of the deformation mode – elastic or plastic – the displacement field must reflect the properties of the force field even if the resulting features may differ considerably in their nature. Therefore it is justified to correlate the properties of the calculated force field with fabric elements observed in plastically deformed rocks. X_1 is the shear zone boundary (Fig.12). Of the eigendirections, *e* is identified as the S-plane in S-C-fabrics[25] and the plane parallel to which the main anisotropy of crystals is oriented. It is thus a stretch-only, no-rotation-no-shear direction. The predicted angle of ca. 11° compares favorably with the obliquity of fabric diagrams from monomineralic shear zones formed of minerals with only one major shear plane (ice, mica).

c is not well developed in high-temperature tectonites. It may be recognized through a lack of pressure shadows, or minimum mica alignment along the surface of feldspar porphyroclasts. However, if mylonites are exhumed they commonly develop joints that cut the layering at ca.70-80°, consistently inclined against the direction of shear. They appear to be controlled by the elastic energy stored during plastic deformation which is released when the confining pressure is no longer able to hold the rock together. This model predicts that dilational cracks should open parallel to *c*.

Considering regional scale, the maximum compressive loading direction along the San Andreas Fault in California is known to maintain an orientation to the fault which is often called perpendicular. The data in Ref.26 show, however, that it is not perpendicular, but commonly at around 80° to the fault, consistently inclined against the sense of

shear (Fig.16). It is, in other words, within limits of natural variation indistinguishable from the *c*-direction of the model presented here. The observed maximum loading direction along the San Andreas Fault has caused puzzlement because it cannot be predicted by the current theory, and is presently the subject of a drilling project.[27] It might be worthwhile to ponder the thought whether this is indeed the Fault's fault, or whether it is rather the theory that is insufficiently understood.

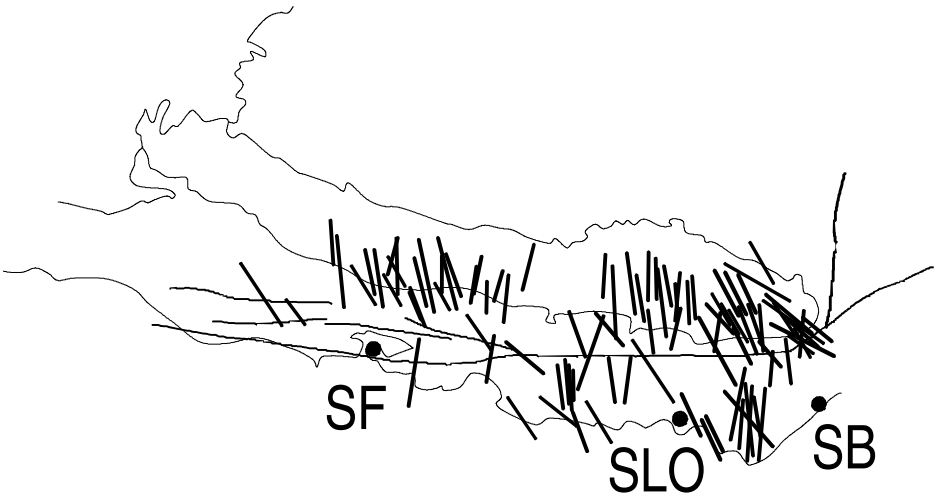

Fig.16 San Andreas Fault System in California, simplified after Ref.26. Thin lines: coastline, and outline of Great Valley. Medium line: San Andreas Fault and other major faults. Thick lines: measured horizontal maximum loading orientations, commonly observed from borehole breakouts. SF: San Francisco, SLO: San Luis Obispo, SB: Santa Barbara. Angular relation of measured maximum elastic loading with San Andreas Fault is within natural variation similar to *c* in Fig.11.

The shear plane at $\theta = -28.83°$ is the Riedel plane R or the C-plane in S-C-fabrics.[28] The P-plane is usually suppressed in natural plastic deformation, but has been observed in shear box experiments, and is occasionally found as a minor shear direction (Fig.11).[29] It is better developed if the *PTt*-conditions were near the brittle-plastic transition zone. The synthetic R-plane (here dextral) and the antithetic P-plane (here sinistral) are not mechanically equivalent. The R-plane is expected to be the first to yield at the onset of plastic flow. Fig.11 shows the flow field. The sense of shear on the R-plane is synthetic to the bulk sense of shear, but the R-plane also simultaneously rotates antithetically towards *e*; in the process it is progressively stretched until it decays. R- and P-planes are stretching faults in the sense of Means.[30] The author believes that this paper provides the theory anticipated by Means for his steady state foliation concept.[31]

8. Energetics of Elastic and Plastic, Pure and Simple Shear Deformation

8.1 Elastic deformation

The state in which the system is, is controlled by the operative force field which serves as

a measure of the field strength. It can be used to compare deformation types with one another. In the elastic mode, the operative and the deviatoric field are proportional to one another during loading; thus they both require work which represents the elastic potential. Since the sum of $\mathbf{f}_{n(dev)}$ from 0 to π is zero, the work done by normal forces is only the work done by $\mathbf{f}_{op}$,

$$\int_0^{2\pi} f_{op} d\theta = -2\pi \tag{49}$$

for $r_0 = f_0 = \Delta f_{op} = 1$ (cf.eqn.21). For an isotropic state, this would be the only term to be considered in 2D; in absolute numbers it turns out the be the maximum work for all states. This work will cause an isotropic contraction. Work done by shear forces will cause a directed dilation. Integrating eqn.29 from 0 to $\pi/2$ for one quadrant, times 4 to account for all quadrants, yields 8.000; total work in elastic pure shear is therefore $w_{PS(el)} = 8 - 2\pi = 1.717$.

In elastic simple shear, the magnitude of $\mathbf{f}_{op}$ is the same as above. The shear work term (eqn.48) must be evaluated for one sector from *c* to *e*, and multiplied by 4 to account for all sectors. Total work in elastic simple shear is thus $w_{SS(el)} = -2\pi + 8.144 = 1.861$. At similar operative field strength, an elastic simple shear thus requires 8.4 % more energy than pure shear.

8.2 Plastic deformation

The mechanism by which plastic deformation is achieved is not in the scope of this paper; however, it is here assumed that the material remains continuous, and that a homogeneous state of the force field **f** is maintained. The transition from the elastic to the plastic deformation mode (the yield point) is marked by a change from reversible to irreversible behavior. Thus the operative field reaches a stable value requiring no more work.

All further work, the plastic deformation energy, is then work done by shear forces only. Since the dilation caused by them is also an elastic feature, the buildup of which stops at the yield point, the energy is not stored in the volume of the system, but dissipated along its surface. Since the system therefore behaves passively, the double shear work concept (see discussion following eqn.29) no longer applies, thus the required shear energy is only half the amount for elastic deformation. Dissipated energy is energy lost and need not be balanced; however, since no free whole-body rotations are possible in a field with real eigendirections – which are still required by the continuing existence of the elastically loaded state – the torque must still be balanced.

For pure shear, the sinistral and dextral shear integrated balance, thus no external rotation of the system is possible. In terms of work done, sinistral and dextral shear work add, thus the work done in plastic pure shear is half of the amount done in elastic loading, i.e. $w_{PS(pl)} = 4$.

For simple shear the affairs are a little more complex. Eqn.46 integrated from the contracting to the extending eigendirection for both sectors yields differing magnitudes: 1.339 dextral shear work in a large sector, and 0.733 sinistral shear work in a small sector.

The imbalance for the entire system is 1.202, the total shear work done on the entire system is 4.144. Since the large sectors dominate, the imbalance is resolved into plastic dextral bulk shear. However, the resolution of the dextral imbalance leads to an imbalance in the torque of the entire system. Since the shape of the system is elliptic and the long axis of the system is in the small sector with sinistral shear, the angular momentum of the system is proportional in magnitude, but opposite in sign to that of the resolved shear, i.e. sinistral. The dextral plastic shear work costs energy which is dissipated, i.e. it is an internal dextral rotation. The rotation of the system due to the angular momentum is an external sinistral rotation which is free. Since internal and external rotation cancel, the eigendirections are still real. Thus the energy dissipated due to a plastic dextral shear is *minimized* by an external sinistral rotation, and the energy thus saved is proportional to the imbalance; thus $w_{ss\text{-}pl} = 4.144 - 1.202 = 2.933$.

At similar operative field strength, a plastic simple shear thus requires 26.7 % less energy than pure shear. Energetic differences of such a magnitude have been observed in experiments; they occurred systematically as a function of the displacement field, and independent of the experimental substance (quartz, salt, gypsum).[32, 33]

The calculated work above applies to homogeneous plastic deformation. The ideal elastic-plastic transition is expected at the point where elastic loading exceeds the strength of chemical bonds. Elastic work is stored in the volume of the system whereas plastic work takes place on its surface. The surface-volume ratio for any given body shape decreases with increasing scale; thus energy will be saved during plastic flow if certain volumes are deactivated, and the actively deforming volume is restricted to a minimum. More energy will be saved if the displacement type within the active regions is a simple shear. This prediction would offer an explanation why a homogeneous elastic pure shear commonly decays into a heterogeneous network of conjugate simple shear zones at the yield point.

9. Properties of Plane Deformation in Three Dimensions

So far, the model was discussed in two dimensions only, ignoring the dimension perpendicular to the kinematic plane. The ambient and the operative field have isotropic properties. Thus they act in all three dimensions, implying that the intermediate direction is not neutral even if the boundary condition (plane strain) stipulates that the finite effect perpendicular to the kinematic plane is zero. This effect is discussed now. – Here, the coordinates x_1, x_3 define the kinematic plane, and x_2 is perpendicular to it.

9.1 Nature of boundary conditions for plane deformation

If work is understood in the Newtonian definition $w = \mathbf{f}\cdot\mathbf{d}$, it is natural that no work is done in directions for which $f_i = 0 = d_i$. Thus it is commonly held that no work is done in directions in which no displacement takes place. This is not correct in the case of changes of state, however.[11, 12] Consider a solid container which is filled with air, and closed by a

piston. If the piston is moved inward the pressure increases; but it does not matter if it is the piston or any other part of the walls that move, or if all the walls move inward – the pressure increases on all the walls. The condition that the walls of the container do not move, is a boundary condition that can only be maintained by increasing the pressure from outside, that is, the non-moving walls do work too. If both the piston and the bottom of the container move at the same rate in the same direction the volume of gas is externally displaced, and Newtonian work is done; but no internal change of state is observed, and no *PdV*-work is done. If a cylinder of solid is shortened in x_3, it will expand both in x_1 and in x_2. This is an effect of the principle of least work: it will require addtitional work to get the stretch in x_2 back to zero if a plane deformation is to be achieved, and even more work if no net change of length in x_3 too is the desired result. Therefore the directions in which no net displacements occur, are nevertheless not "dead" directions. The situation is complicated by the fact that a gas can only be in an isotropic state of static loading whereas solids can be loaded anisotropically, and two different loaded samples with similar volume may be in two energetically different states of loading nevertheless.

9.2 Forces and displacements in plane deformation

Consider a system in a large continuous body of solid subjected to plane deformation external conditions. The contracting eigendirection *c* will be in x_3, the extending eigendirection *e* is in x_1, and no net change is to occur in x_2 which is the intermediate eigendirection. The forces which act upon a system of solid in a continuum are (eqn.18):

$$\mathbf{f}_{\text{total}} = \mathbf{f}_{\text{op}} + \mathbf{f}_{\text{dev}} + \mathbf{f}_{\text{s(int)}} + \mathbf{f}_{\text{s(ext)}}$$

where the force field $\mathbf{f}_{\text{op}}$ is always isotropic and inward-directed, representing the ideal change of state; the deviatoric field $\mathbf{f}_{\text{dev}}$ is decomposed into the normal components $\mathbf{f}_{\text{n}}$ and the shear component $\mathbf{f}_{\text{s(ext)}}$; and due to the bonded nature of the contact of system and surrounding there is an extra shear force component $\mathbf{f}_{\text{s(int)}}$ (cf. text following eqn.29). Thus a contraction in x_2 is caused by $\mathbf{f}_{\text{op}}$.

Take pure plane shear as an example, where the extending eigendirection *e* // x_1, the contracting eigendirection *c* // x_3, and x_2 is the intermediate eigendirection in which no finite deformation is observed. Altogether, the force along the main directions are composed as follows: in x_3 there are 1 $\mathbf{f}_{\text{op}}$ +1 $\mathbf{f}_{\text{n}}$ = 2 inward-directed components. In x_1 there are 1 $\mathbf{f}_{\text{op}}$ - 1 $\mathbf{f}_{\text{n}}$ - 1 $\mathbf{f}_{\text{s(int)}}$ - 1$\mathbf{f}_{\text{s(ext)}}$ = -2 outward-directed components. In x_2 there is 1 $\mathbf{f}_{\text{op}}$, but the normal deviatoric force acting on the system is zero since in x_2 there is only the ambient (pre-loading) and the operative field. The component $\mathbf{f}_{\text{s(ext)}}$ is zero too, so only the system shear component $\mathbf{f}_{\text{s(int)}}$ is present since the boundary conditions permit the system to expand by itself, resulting in 1 $\mathbf{f}_{\text{op}}$ - 1 $\mathbf{f}_{\text{s(int)}}$ = 0 total force in x_2 (Fig.17, left panel; sign convention: inward-directed components are positive). Thus along x_2, the volume contraction caused by $\mathbf{f}_{\text{op}}$ is exactly cancelled by the system shear dilation. However, although the volume contraction by $\mathbf{f}_{\text{op}}$ and the shear-caused dilation cancel in this example, there is an important difference between the two. The contraction by $\mathbf{f}_{\text{op}}$ is isotropic, thus it does not have discrete eigendirections. In contrast, the dilation by $\mathbf{f}_{\text{s}}$ is

anisotropic, a stretch is observed both in x_1 and in x_2.

This configuration of forces (or displacements, applying the work function eqn.21) is stable and represents the loaded equilibrium state as long as no bonds are broken, and it remains stable if the system is elastically unloaded. But bonds will be broken if the solid reaches its elastic limit. The orientation of the joint can be expected to be such that maximum energy is released, it should therefore be controlled by the orientation of the eigendirections of $\mathbf{f}_{total}$. But since $\mathbf{f}_{op}$ is isotropic, it can be discounted. We are left with the properties of $\mathbf{f}_{dev}$, i.e. the shortening direction x_3 and two differential extending directions x_1 and x_2. The forces in the latter two cannot be released completely by a defect of any geometric shape because neither a spherical cavity nor a planar crack completely matches the properties of the force field. In order to release the maximum elastic deformation energy (so that the solid can assume its minimum energy state), the maximum extending force in x_1 can only be combined with the one either in $+x_2$ or $-x_2$, ditto for $-x_1$. The deviatoric stretch ratio in the two directions is $\mathbf{f}_{dev}(x_1) : \mathbf{f}_{dev}(x_2) = 3{:}1$. This ratio is interpreted to be the tangent of an angle since it can be >1, and because shear forces are involved. Thus the angle of maximum energy release measured from x_1 is $\pm$ atan 1/3 = $\pm$ 18,44° (Fig.17, right panel). These directions are considered the metastable extending eigendirections e' of the resolved state. They are expected to be perpendicular to the joint planes which also contain x_3; their orientation is thus fully determined, and a conjugate set of joints enclosing an angle of ideally 143° is predicted.

For simple shear, essentially the same orientations are expected, except that the contracting and extending eigendirections are inclined against the sense of shear (Fig.18; cf. Figs.11 & 12), and the angle enclosed by the joints may be larger because the dilation in plane simple shear is larger than in plane pure shear. The predicted joint orientations compare favorably with features observed in the field, both in geological shear zones (personal observation) and in ice (Fig.19).

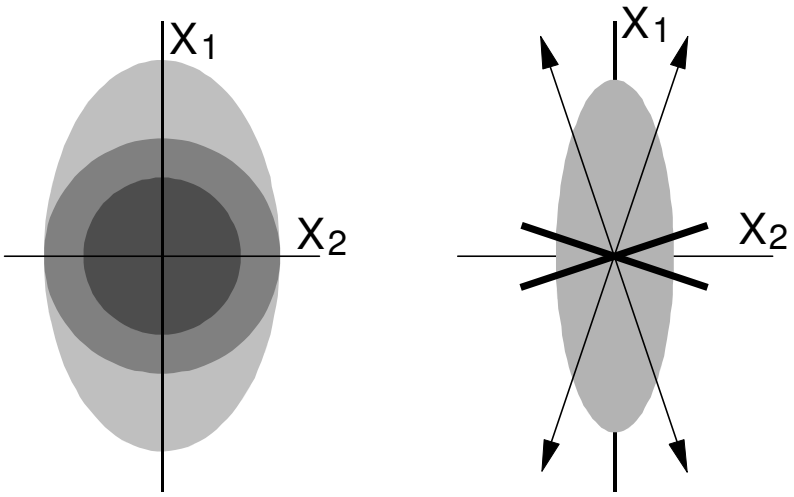

Fig.17 Forces in the x_1x_2-plane in plane pure shear. Shortening direction x_3 perpendicular to page. Left panel: medium grey – outline of thermodynamic system before loading; dark grey – isotropic contraction due to $\mathbf{f}_{op}$; light grey – final shape due to normal forces in x_1, and dilational effect of shear forces in x_1 and

x_2. Right panel. Effect of deviatoric forces only, magnitudes of eigendirections of ellipsoid: x_1: 1 $\mathbf{f}_n$ + 2 $\mathbf{f}_s$, x_2: $^2/_2$ $\mathbf{f}_s$. Combined effect of forces along x_1 and either x_2 or $-x_2$ results in conjugate maximum energy release directions (arrows) and joint orientations perpendicular to them (heavy black lines).

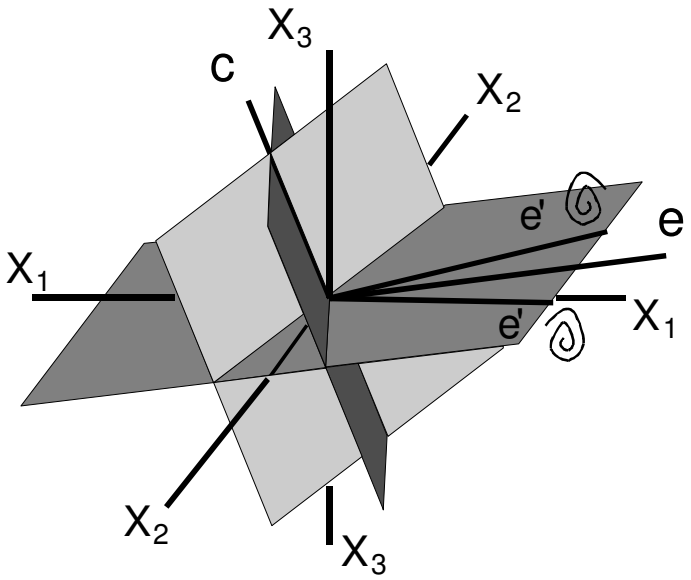

Fig.18 Orientations of joints in space, dextral simple shear. x_i: external coordinates; *e*: extending eigendirection, stable for equilibrium state (elastic loading); *c*: contracting eigendirection; *e*': metastable extending eigendirections for non-equilibrium state (cracking, viscous and plastic flow); spirals indicate opposite sense of unbalanced rotational momentum. Medium grey plane containing x_2 and *e*: S-plane in SC-fabrics; light and dark grey planes containing *c*, and perpendicular to the *e*': joint planes. Bulk foliation plane is x_1x_2-plane.

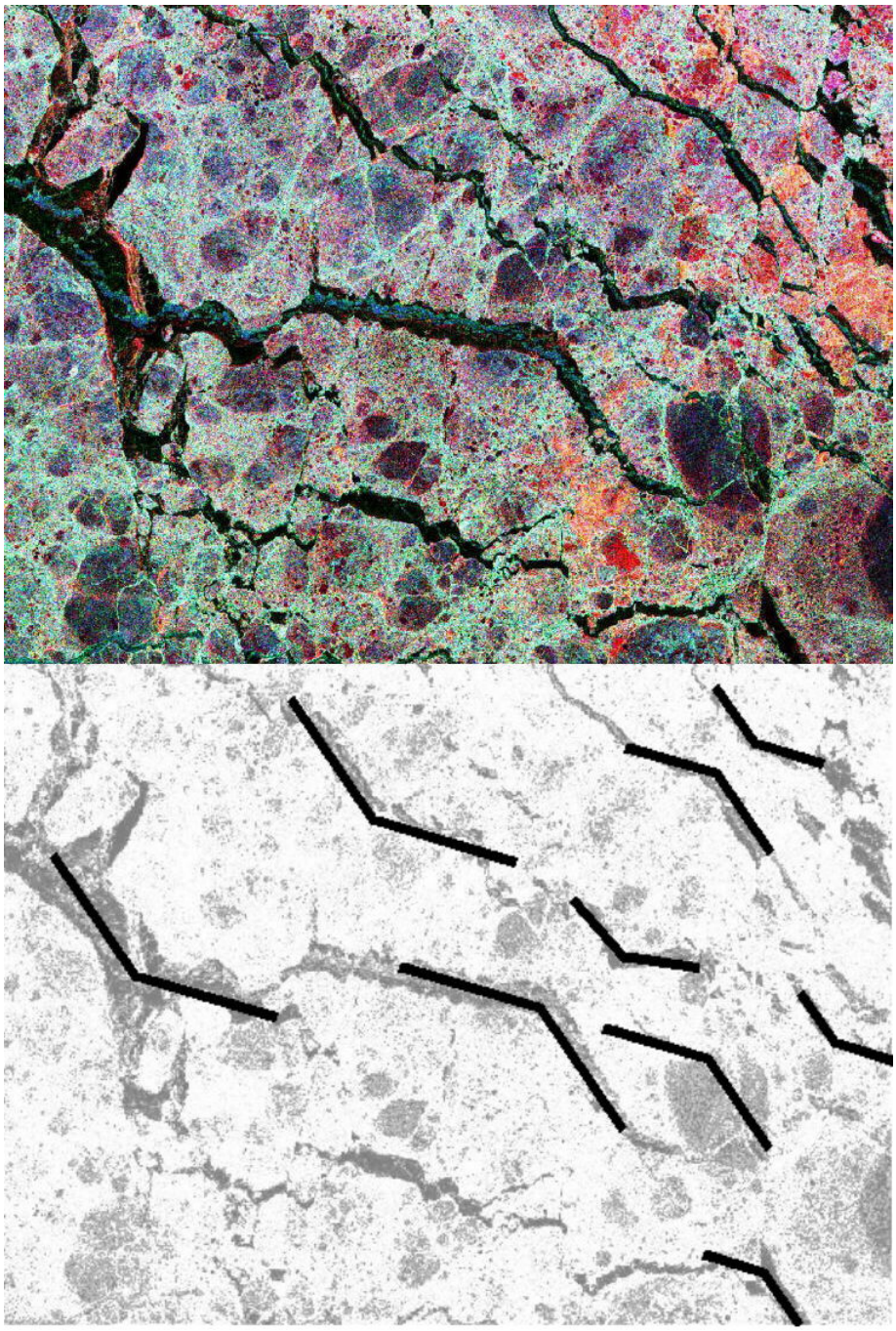

Fig.19 Wedell ice shelf, colors indicate ice thickness. Dimensions ca.40×30km. Ice floating on water is pulled apart by the prevailing wind, opening long cracks (‘leads’). Deformation conditions assumed to be close to plane deformation, with stretch direction oriented NE-SW if vertical image dimension is N. Bottom: the angle predicted in Fig.17 fits well on most natural angles here, with very little natural variation. Nasa image; http://visibleearth.nasa.gov/view_rec.php?id=451.

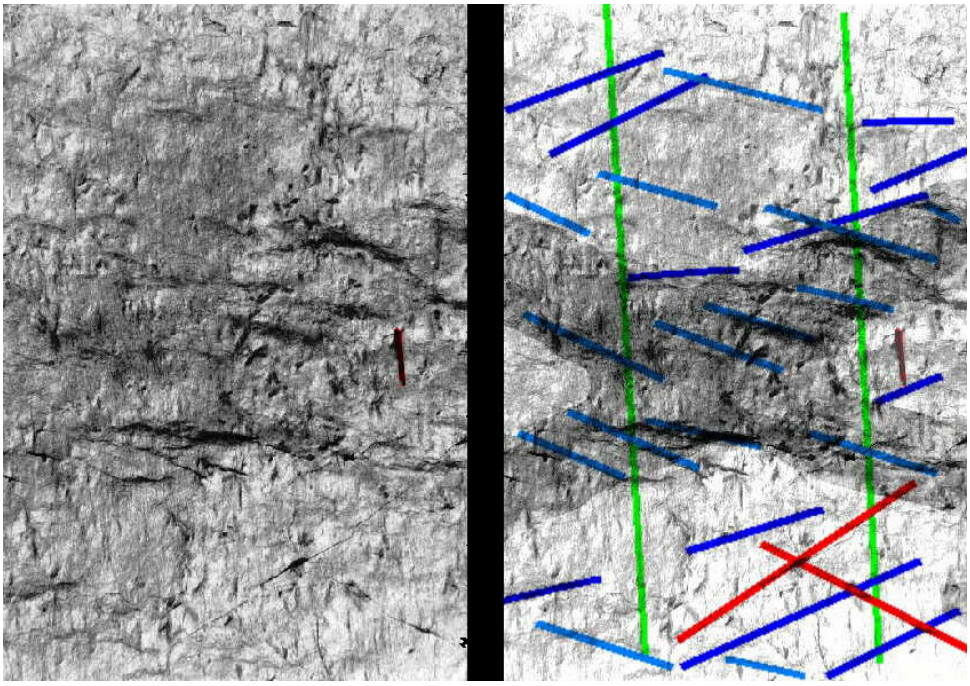

Fig.20 Pelitic schist, view on the foliation plane. Left: Dark elongated spots parallel to lineation: staurolite crystals, red: pen for scale. Right: Structural interpretation. Green: stretching lineation; red: two late joints; blue: traces of C-planes on main foliation (S-plane) form conjugate sets, symmetric relative to lineation; characteristically, one of the sets (light blue, plunging to right) locally dominates over the other (dark blue, plunging to left). The strongly developed intersection structures are substructures of C-planes at a larger scale, two of which, again conjugate, intersect in the picture (darker shaded cross). Note rhomboid structure just above pen due to interference of both SC-intersection directions. – Joints (red), traces of C-planes (light and dark blue) and C-planes at larger scale (shaded) are all conjugate, and symmetric relative to the stretching lineation (green); the plastic structures (C-planes at small and large scale) show the angle predicted in Fig.17. Shear sense revealed by top-bottom asymmetry of small structures is background up, observer down. Gove Formation, Rt.101, New Hampshire, USA.

The model is interpreted to indicate that upon initiation of irreversible processes, started by breaking of bonds (permanent or other), the thermodynamic system of the balanced state decays into two subsystems. However, the release of the deviatoric force field is necessarily lopsided (either $\mathbf{f}_{dev}$ along x_1 and $+x_2$, or those along x_1 and $-x_2$) which has the effect that e is reoriented into either metastable eigendirection e'; that is, for the subsystems the rotational momentum is no longer balanced because bonds are broken. The two sets of subsystems should be rotationally accelerated about c with mutually opposite sense of rotation. The decay of e into e'_{left} and e'_{right} represents a bifurcation event.

In principle, the imbalance indicates that x_2 is not a stable direction in any type of irreversible flow even in plane deformation, and fabric elements or mesoscopic structures parallel to x_2 are subject to reorientation and/or decay. However, the phenomenon caused by the imbalance may differ in nature, depending on the properties of the flowing

substance. Silicate rocks commonly retain a state of elastic loading which has been stored during metamorphic conditions. Once the rock approaches the erosion surface during uplift to the degree that the reduced confining pressure is no longer able to balance the elastically stored energy it may crack. Commonly the coherence is not completely lost, and the released rotating momentum is instantly balanced by external constraints on a larger scale; the conjugate joint set is all that gives witness of the phenomenon. However, if particles spallate off the free surface of a loaded body of solid, there are no longer any external constraints, and the freely rotating shards can be very dangerous.

In highly viscous materials undergoing plastic flow, external rotational acceleration of subvolumina is again prevented by the overall coherence of the material, and disequilibrium can only be local. Yet reorientation may take place at the scale of a grain, or it may be regionally partitioned at varying scale. For example, wholesale reorientation of fabric elements is commonly observed in simple shear zones which have undergone very large finite deformation. Pre-existing passive marker layers are deformed into cylindrical folds, their fold axes are believed to nucleate parallel to x_2. But they are reoriented with progressive deformation to be aligned with the direction of transport x_1 from either side (Fig.21). The resulting structures are called sheath folds because the marker layers form (in the simplest case) elliptical tubes extending parallel to x_1 which are characteristically closed on one side.[34-36] (This author would contend that the fold axes do not nucleate parallel to x_2, but perpendicular to either e'; but the two options will be hard to discern in the field because they will begin to be reoriented soon after nucleation.)

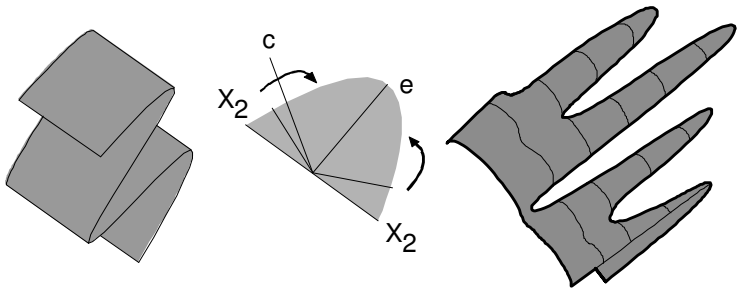

Fig.21 Development of sheath folds. A passive marker layer originally warped in cylindrical folds (left) with fold axes parallel to x_2. During progressive deformation the fold axes will bulge and protrude rodlike into the extending eigendirection e until a strong linear fabric is formed (right). Center: e-x_2 plane: fold axial plane; c: contracting eigendirection. Arrows indicate sense of reorientation of local fold axes.

In materials with low viscosity the coherence may be relaxed to such a degree that external rotational acceleration is indeed possible. Air undergoing simple shear while flowing along an x_1x_2-surface (Couette flow) commonly develops turbulences, i.e. eddies which rotate in either sense about an axis which is close to x_3. Since flow has been considered a conservative physical problem, and since elastic deformation has not been properly understood as a change of state,[11, 12] irreversible relaxation of the elastically loaded state has so far not been considered in the search for the origin of turbulent flow. However, it should be readily recognized as the cause of "elastic turbulence".[37, 38] There is

no obvious reason why the same mechanism cannot work in low-viscosity gases.

10. On the Flow of a Real Gas

The force in Newton's equation of motion $\mathbf{f}_V = m\mathbf{a}$ is a *single-vector force* by nature, with unique direction and magnitude. It describes the acceleration of a discrete body in freespace due to collision with another body. This restricts the applicability of $\mathbf{f}_V$ to conservative environments where the conservative law of energy conservation $E_{kin} + E_{pot} = const$ applies; beyond that it is of phenomenological value only. $\mathbf{f}_V$ cannot be derived, and it cannot form a field. The force $\mathbf{f}_F = \mathbf{e}_i \partial U/\partial x_i$ is a *field force*, indicating that relative to some reference point Q, to every point in space with position vector $\mathbf{r}$ a vector $\mathbf{f}$ can be assigned through a function $\mathbf{Tr} = \mathbf{f}$ where $\mathbf{T}$ is the field property tensor. This definition is far more general; $\mathbf{e}_i \partial U/\partial x_i$ is not an equation of motion. Whether an observed force is of type $\mathbf{f}_V$ or $\mathbf{f}_F$ must be decided by inspecting the physical problem under consideration. The two types of forces differ profoundly in their physical and mathematical properties, they cannot be transformed into one another.

All free atoms in a gas are subjected to two sets of forces. (1) Atoms travel at some finite speed and undergo positive or negative acceleration during a collision. (2) Atoms carry with them an electromagnetic field which attracts or repels other atoms. In the theory of gases the latter is usually ignored, as e.g. pointed out by the cautionary remark of Döring (Ref.39, p.12) "*If* the assumptions of our model are correct [...] that the mean potential energy of the interactive forces (among the atoms) can be ignored in relation to the kinetic energy (of the atoms) ..." The assumption appears to be justified at first sight because the mean velocity of atoms in freespace at room temperature is in the order of 500 to 1000 m/sec (Ref.39, p.12), and the electromagnetic potential is assumed to be of importance only at very close range.

However, the nature of both forces involved differs profoundly even though their effect may be similar to some extent. Consider some confined volume V with surface A containing one atom. In order to exert a pressure on the surrounding in all directions, the atom must bounce around and exert a force $\mathbf{f}_V$ such that all points of A are touched, which is possible only over infinite time. The required time Δt may approach zero as the number n of atoms in V is increased towards infinity, but it cannot reach zero. In contrast, even the force field $\mathbf{f}_F$ exerted by one atom is felt at all points of A simultaneously at $t = t_0$.

The natural atomic velocities above are at least ten times as high as those of the most devastating hurricane. The macroscopic diffusion rate in a gas is seven orders of magnitude lower; this gives a measure as to which degree an initial signal (momentum) can be changed by ca. 10^{10} interatomic collisions per atom per second. Assuming that the atoms behave like spherical bodies, the travel direction of one particular atom becomes unpredictable after a very short time. That is, the combined effect of $\mathbf{f}_V$ of all atoms is random at the atomic scale, and isotropic at the scale of V, and this condition is rather stable: whatever external influences exist which could superimpose some order on the random motions to create a form of homogeneous atomic flow, will instantly be wiped out. It is therefore hard to see how an external mechanical momentum – either single, or

in the form of a momentum front – can propagate through a gas at a speed appreciably faster than the diffusion rate, and without loosing its direction. Wholesale acceleration of a volume of gas by a spatial array of $\mathbf{f}_V$ (avoiding the term *field*) causing a directed, systematic acceleration of n single atoms moving in n different directions is therefore not possible; and if it were possible, the macroscopic flow velocity would have to approach the natural atomic velocities with increasing geometric order. However, such velocities are not observed. Homogeneous flow at the macroscopic scale exists apparently despite the random motion at the atomic scale, i.e. the two processes take place simultaneously and – to a first approximation – independent of one another. This implies that it must be possible to cause whole bulk volumes of a gas to flow in a regular way at the macroscopic scale without support or interference by the motions at the atomic scale.

(Stokes[40] did consider random motions of atoms in a gas and believed that his theory should be valid on the macroscopic scale nevertheless. His theory comes apart because the natural atomic velocities are far higher than he imagined. The natural velocities were already predicted in the 19th century, but not believed; they were shown to be real only in the 1920s.)[39]

If it is not the individual atoms which are made to flow in a systematic pattern by an array of external momenta, it is useless to start the theory of flow with an equation of motion. Instead, the evidence calls for a mechanism which is independent of kinetics. The key to understand flow of a gas must therefore be in the existence of the field forces $\mathbf{f}_F$ which have their origin in the electromagnetic potential energy U_{em} of the atoms (cf. eqn.2 and eqn.4a). Kinetic energy E_{kin} is exchanged only during mechanical collision of atoms and causes a gas to fill a given V homogeneously by maximizing disorder. Field forces $\mathbf{f}_F$ are felt over long distances in freespace, and they are *attractive*, i.e. even if they are much smaller than $\mathbf{f}_V$ they have the potential to bring about a least energy configuration, thereby reducing randomness. Thus $\mathbf{f}_V$ are now ignored. Due to $\mathbf{f}_F$ there must be a spatial energetic structure even in a gas, and that structure is isotropic in the static state.

One consequence is that the atoms can no longer be considered discrete bodies in freespace. A body is said to be discrete if it is possible to envelop it by a closed surface A such that no point in A runs through mass;[7] only then is it permissible to reduce the body to a point source (i.e. ignoring its volume, and considering the entire mass of the body to be concentrated in one point; points on A are neither system nor surrounding since both reach inifinitely close towards A). The condition is meant to clarify whether work done by a given mass quantity is part of the work done by the surrounding on the system or vice versa. If atoms can be considered discrete bodies in freespace, their motion is holonomic, i.e. unrestricted in the sense that the motion of one particular particle does not implicitly affect the trajectories of all others. But bonds are field forces $\mathbf{f}_F$ which can do work at long range, and the motions of bonded atoms are not holonomic. At time scales which are short in comparison to the diffusivity, the random motions must be disregarded altogether, and the gas acquires properties similar to those of an elastic solid since its energetic structure defines its mechanical properties, and the average distance between an atom and its neighbors is optimized. Only if such a structure exists, the gas is able to build up an elastic potential; after all, elastic work is work done by changing bond lengths, not by displacement of mass in freespace, and the best evidence for elastic deformation of a gas

is the transmission of sound. Thus Kellogg's statement must be extended to the effect that the freespace condition does not hold if *A* dissects an energetic bond, be it transient as in a gas, or permanent as the chemical bonds in solids. The material, be it a gas or a solid, is therefore no longer a kinetic system of *n* discrete bodies, but it represents a homogeneous mass distribution with the potential to act as a mechanical lever. – The problem relates to the question how a minimum thermodynamic system is to be chosen in a real substance. It could be chosen so that *A* encloses one single atom, cutting through the bonds with its neighbors, or vice versa it could be chosen to enclose the bonds, cutting through the atoms. The former appears to be the more natural choice, but for the latter there is a precedence case – the minimum lattice cell in crystallography which must contain the bulk composition, and which has atom fractions at its corners. If the latter is the correct choice, Kellogg's requirement is unambiguously answered because in that case *A* does run through mass.

Since a least-energy structure exists in a gas it can be perturbed. The propagation of the information that a perturbance occurred, is not bound to mechanical interaction, but it is transmitted by field forces, and will proceed at the speed of sound through the gas. In principle, the reaction of a gas to anisotropic loading should be similar to that of a solid as long as time-dependent processes can be ignored. In that sense the deformation theory outlined in this paper should apply to the flow of fluids too, including the bifurcation at the reversible-irreversible transition explained above. The suggestion is supported by observations since a gas has the same propensity to concentrate deformation in narrow shear zones as a solid undergoing plastic flow. In Fig.22 air passes through a tube. The center of the stream expands homogeneously parallel to the tube, but apart from that it remains largely undeformed. Active flow is restricted to a very narrow band near the walls. These zones deform by simple shear (called Couette flow in fluid dynamics), and they are also zones of reduced mass density, relative to the center of the stream at similar distance from the tube exit. The evidence suggests that regions actively deforming by an irreversible process such as viscous flow are minimized whereas regions which are passively translated are maximized. Apparently this partitioning requires less energy than homogeneous flow. The observation is in agreement with the prediction that irreversible simple shear flow requires substantially less work per unit strain than pure shear, and that zones undergoing simple shear are measurably dilated elastically relative to a continuum at rest (above). Also, the expansion in the center of the flow is not isotropic since boundary conditions permit expansion only parallel to the tube. Thus the bifurcation may be triggered inevitably at some point in time not only in the boundary layer, but in the center of the flow itself. Again, this is in agreement with experimental observation showing that turbulence is impossible to avoid even under maximally ideal conditions.

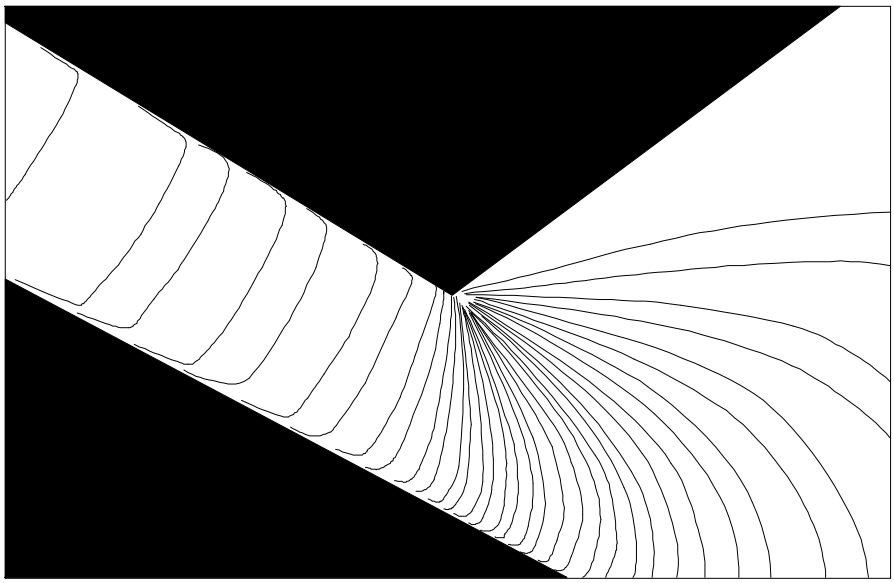

Fig.22 Mach-Zehnder-inferogram of air flowing through a tube and past an opening. Equidensity lines indicate gas inside tube homogeneously expanding towards the exit. Very low density gradient perpendicular to tube in center of flow, strong density decrease in thin layers near walls (known as Prandtl boundary layer). Redrawn after Ref.45 (original figure from Ref.46).

The entire internal energy U_{int} of a volume of gas thus consists of two components (Ref.11, eqn.2): the kinetic energy E_{kin} of the n atoms in the system, and the electromagnetic field energy U_{em} from which the force field $\mathbf{f}_F$ is derived (Ref.41, p.37). It can be assumed that $E_{kin} >> U_{em}$ in a gas, but an elastic deformation can only cause a change of U_{em}; E_{kin} can only be changed through atomic collisions (change of the average velocity would amount to influx of heat) the spatial effect of which is isotropic. Thus a change of state ΔU_{int} due to the elastic deformation is a change of U_{em} (Ref.11, eqn.4a). Consider a volume-constant elastic deformation of a gas. It differs from the undeformed state only in that it is ordered. Consider a volume of space with an atom in the center at t_0, and with a radius proportional to the mean free distance in all directions. In the unloaded standard state the shape of the volume element is isotropic-spherical, and collisions will take place in all directions at t_1. In the isochoric deformed state the shape is that of an ellipsoid, and its eigendirections and its orientation in space are those of the displacement field. Between t_0 and t_1 the velocity structure becomes anisotropic since the collisions parallel to c will occur earlier than those parallel to e; consequently, scattering will cause a momentary preference for the velocity vectors to be aligned with e. The anisotropy will be dissipated after a few collisions unless the loading is continuously renewed through external control such that the dissipation rate equals the loading rate per unit time. When the stored energy ΔU_{em} is dissipated, the ordered state disintegrates at constant volume, and ΔU_{em} is converted into E_{kin} by diffusion and hence into heat. Given the difference in magnitude of U_{em} vs. E_{kin} the thermal effect of the dissipation of ΔU_{em} is expected to be small, but not zero.

If the proposition made in this paper is accepted that flow of a gas is not due to mechanical interaction of individual atoms in the sense of Newton, but due to electromagnetic-thermodynamic force fields and interaction of system and surrounding, it would relieve theoretical thinking of the restrictions inherent to kinetic concepts, especially the necessity to know both location and velocity of the atoms in the initial state; it is not possible anyway.

11. The Navier-Stokes Equations

The basic tool in the understanding of fluid dynamics to date is the set of Navier-Stokes equations. Although they have been in use for 160 years it is amazing to see how little is really known about them. It is not even known whether solutions to the Navier-Stokes equations actually exist, or whether the vector field exists which is implied in the equations.[42] For the so-called incompressible flow the equations are

$$\frac{\partial}{\partial t}u_i + \sum_{j=1}^{n} u_j \frac{\partial u_i}{\partial x_j} = \nu\nabla^2 \cdot u_i - \frac{\partial P}{\partial x_i} + f_i(x,t) \tag{50}$$

$$div\, u = \sum_{i=1}^{n} \frac{\partial u_i}{\partial x_i} = \nabla \cdot u_i = 0 \tag{51}$$

where $u = u(x, t)$ is the velocity vector, $f = f(x, t)$ is an external force, P is the pressure, and ν is the viscosity coefficient. Eqn.50 is just Newton's law $f = ma$ for a fluid element subject to the external force f and to the forces arising from pressure and friction. If $\nu = 0$, eqns.50 and 51 are also known as Euler equations.

As pointed out earlier, much confusion in the thinking on deformation and flow stems from inappropriate terminology.[12] What is meant by "incompressible flow" is actually volume-constant flow and a boundary condition; "incompressibility" implies a material property that does not exist in nature. Furthermore, P is commonly and correctly understood to be a state function; but if $P = \partial U/\partial V = const$, the rest of eqn.50 suggests that "incompressible flow" is conservative, and no change of state is involved (Ref.43, p.142-144; Batchelor actually considers that P is not to be understood as a state function, but leaves open what then it should be). However, the mass density is not a state function in anisotropic loading because volume-neutral elastic deformation clearly is a change of state: work is done upon a system such that its internal energy changes, and an elastic potential builds up.

The first, second, third, and fifth term in eqn.50 are conservative and relate to Newtonian mechanics (for discrete bodies in freespace), including Newton's third law as equilibrium condition (that forces acting on some body must balance), to a velocity potential, and to Bernoulli's energy conservation law exclusively; whereas ν in the third term refers to an irreversible, hence to a non-conservative process, and the fourth term is a thermodynamic one, non-conservative by nature, referring to the thermodynamic equilibrium condition (that forces exerted by a system on the surrounding and vice versa must balance).

Eqn.51 was meant to be a conservation law for mass and momentum. It is

conservative in mathematical structure, and supports the Newtonian nature by which fluid flow was so far understood. Eqn.51 asks the wrong question; instead of mass, it is the energy balance that needs to be considered which is non-conservative. Moreover, fluid flow is an irreversible process, hence it involves production of entropy. Trying to find a conservative approach to a dissipative process can at best result in a phenomonological solution, but it cannot lead to proper understanding.

Stokes[40] was already contradicted 25 years later by Clausius[20] who identified the kinetic energy in the equation of state – that is, the only term to which a Newtonian equation of motion is relevant – as the heat term (Ref.11, first term LHS eqn.4a), leaving work due to elastic effects to be done by the surrounding. The difference in the thinking of Stokes and Clausius is most sharply juxtaposed in their respective equilibrium conditions: Stokes used Newton's third law, whereas Clausius used the thermodynamic equilibrium condition.

Apart from that, the derivation of the Navier-Stokes equations is so heavily based on the existence of the Cauchy stress tensor (e.g. Ref.43, to name just one example) that they must necessarily fall with it. The postulated force field $\partial u_i/\partial t$ cannot exist. $\mathbf{f} = m\mathbf{a}$ is not and cannot be a vector field, it is one single vector only. Viscous flow is not a conservative physical process, and an equation of motion does not help. A proper equation of state is needed, and a viscous flow step must be decomposed into (1) a reversible, time-independent, elastic loading step and (2) an irreversible, time-dependent, diffusion-controlled relaxation step. Thus phenomena should be observed in gas flow which may derive both from elastic-reversible as well as from viscous-irreversible aspects of the problem. This is indeed the case (Fig.22).

The mentioned decomposition is anything but novel. It was proposed by Poisson ca.1830 and known to Stokes[40], he and this author merely differ in the conclusions: Stokes believed that his theory was fully compatible with Poisson's proposition whereas this author believes that he missed the point. But he is in good company, Poisson missed it too. It is unfortunate that Stokes published his theory in 1845, three years after Mayer had discovered the First Law of thermodynamics, and two years before Helmholtz discovered it again, making it finally become common knowledge. Only from then on the full tool box of thermodynamic concepts, including the strict separation of system and surrounding, the importance of the equation of state, the difference between Newtonian work and PdV-work, and mundanely the difference between Newton's 3rd law and the equilibrium condition of thermodynamics became appreciated. Also, it is highly ironic that Poisson himself did much to confuse the understanding of elastic deformation by introducing the ratio ν named after him – it is entirely phenomenological, dependent on specific boundary conditions, not at all a material property, and helped to keep thinking about elasticity solidly on the wrong track; whereas Poisson never knew that he had indeed discovered the real key to understand elasticity – his equation, $\nabla^2 U = \varphi$. It makes the observer feel humble; we are all children of our own time.

12. Application to a Discrete Body Problem

Up to this point, the assumption had been made that the system is part of a much larger space of homogeneously distributed and bonded mass, and any boundaries to freespace are infinitely far away (ideal continuum model). Here, the theory is applied to model the loading conditions in a discrete body with given shape subjected to a loading configuration that includes interfaces to freespace.

The Euler-Cauchy theory is inconsistent in its reference to distances in real space. On the one hand, a unit length l_0, e.g. the length of the spring in Hooke's law, is readily used to define a relative change of length Δl; on the other hand, through Cauchy's "continuity approach", the reduction of a volume element with surface facets into Euler's group of planes passing through one common point, the measure of spatial extent of the volume element was lost.[9, 11] In thermodynamics this distance term is the radius of the thermodynamic system which is finite. For this reason the theories of continuum mechanics and thermodynamics are incompatible. This fact itself has been noted before by others, but not the cause.[6, 44] In potential theory this basic distance in real space is called the zero potential distance for which Hooke's l is a good example. The absence of this distance term made the Euler-Cauchy theory rather cumbersome to apply, indeed it was necessary to re-invent the term and fudge it back into the theory. The result was the finite element method which uses a grid of predetermined points or nodes for which solutions can be found, and the distances between the nodes act as local unit distance l. The number of nodes grows exponentially if more detailed solutions are needed. The real problem is, however, the Euler-Cauchy theory is not a proper field theory because it was not derived from a potential which provides a scalar field to start from. A field theory delivers a solution for the entire region for which the set-up is defined. It may may then be solved numerically for any point within that region. A grid of nodes is unneccessary.

A big issue in the Euler-Cauchy theory is the continuity condition. This is highly misleading. Euler's continuity condition is really a law for mass conservation. But mass conservation is not a problem in thermodynamics, it can be excluded by assuming that the system is closed with regard to mass fluxes, then all attention is paid to energetic fluxes. Within the elastic realm, mass may expand or contract while bonds remain continuous. If any continuity is of interest in the mechanics of solids it is not so much the continuity of mass distribution which is easily checked, but the continuity of bonds; this is a boundary condition. But bonds were never considered in continuum mechanics.

The approach applied here is based on potential theory. The thermodynamic continuum is not a continuum of points, but a continuum of systems. Any point Q in Euclidean space within a region of distributed mass can be thought to be the center of mass of a thermodynamic system; its physical properties – density, chemical composition, temperature, material properties, orientation of anisotropy – plus those of the external boundary conditions are then functions of Q. Scale independence ensures that the extensive properties are scaled per unit mass (mol, not kg). Thus two infinitesimally close points Q_1 and Q_2 represent two different thermodynamic systems V_1 and V_2 of some finite unit size; they largely overlap, but their physical properties or boundary conditions may be subject to gradients in Euclidean space. The systems may be understood to have unit mass, unit volume, or unit radius which are all finite. The radius, missing in the Euler-Cauchy approach, therefore offers itself as the base of a wave function. The spatial

distribution of physical conditions can thus be modeled as a function of the boundary values through a Fourier series approach.

12.1 Forces and boundary conditions

Work in the bonded continuum differs from Newtonian work in its spatial effect. Newton's $\mathbf{f} = m\mathbf{a}$ is one single vector, it cannot be a vector field; thus $w = \mathbf{f} \cdot \mathbf{d}$ is simply the work done in displacing a body of mass m by a distance $\mathbf{d}$. In contrast, it is not possible to do work in only one direction in a continuum.[12] In many textbooks a cylinder of length x filled with air and closed with a piston is used to explain the concept of work: if x is changed by moving the piston, the pressure in the gas is a function of Δx. The example is misleading; it is not just the piston that does work on the gas, but also the walls of the cylinder which do not move. Without them the pressure could not increase because only externally balanced forces are able to cause a change of state, and for the change of pressure *per se* it does not matter if only the piston, or all the walls move. The 'ideal change of state' leading to the isotropic operative field (eqn.18, fig.2) was introduced to avoid this spatial interdependence in the first step. Of prime interest are not the displacements of the walls, but the change of state which surely is done evenly on all of the gas in the cylinder. Thus if spatial boundary conditions exist, attention must be paid nevertheless to those directions in which apparently nothing happens according to the boundary conditions. It is not helpful to think in terms of displacements primarily; it is the forces that are the cause of deformation. The displacements are the effect, they are found in the end through the work equation.

The total force field is partitioned into the isotropic operative force field $\mathbf{f}_{op}$ and the deviatoric force field $\mathbf{f}_{dev}$ (eqn.18). The latter can again be decomposed into the normal component $\mathbf{f}_{n(dev)}$ and the shear component $\mathbf{f}_{s(dev)}$. Normal forces will shorten or stretch the radius vector on which they act, depending on sign; shear forces will always have a dilating effect; which amounts to an additional stretch component parallel to the extending eigendirection e. Following eqn.29 it was stated that the work done by shear forces counts twice because one part of the stretch due to shear dilation in e is done by the system itself, the second part is done by the surrounding. The component originated by the system is purely a function of the loading configuration, it will happen if the system is given the freedom to expand by the boundary conditions. The shear dilation which is caused by the surrounding, however, depends on the existence of the surrounding and/or the bonding across system-surrounding interface. In a perfect continuum it surely exists, but its effect must reach zero at the interface to freespace. If all other possible variables are kept constant it is this component that must vary as a function of location within a body, i.e. it is sensitive to the body shape and the specifics of the loading configuration.

The 2D-model consists of a rectangular body of solid. It is thought to be loaded on top and bottom with constant force whereas the lateral faces are free. The applied load is vertical, or parallel to y ($df_y/dx = 0$). The loaded faces ($y = 0$, $y = 1$) may not change length in x due to friction at the pistons; at all other y they are free. Thus the load is the same throughout the body, there is no gradient. This includes the points on the lateral

faces. Consequently the magnitude of the operative field $\mathbf{f}_{op}$ and the normal force field $\mathbf{f}_{n(dev)}$ are monotonous throughout the body. They are not included in the model here.

The boundary conditions in the regions near the loaded faces cause the material to undergo some real volume contraction. Unsurprisingly, they are mechanically in a very stable condition although they are the regions with maximum energy stored per unit volume. Gradients in stored energy are due to the ability of the material to dilate, as a function of the boundary conditions. A map of energy stored and a map of dilation permitted will not be identical, however, because dilation is always an energetic relaxation from the maximum load. Thus the regions of maximum energy stored and maximum dilation allowed will differ. The latter is of greater interest, however, it can be called the failure potential, so the model concentrates on this aspect.

The boundary conditions for the dilational shear T vary over the body in a two-fold way: (1) the restriction of no change of length in x suppresses even the dilational effect produced by the system (system effect, T_1), it is strictest along the loaded faces $y = 0$ and $y = 1$, and relaxes towards the center of the solid, allowing for progressive expansion in x; and (2) the shear effect produced by the surrounding (surrounding effect, T_2) is fixed to a given minimum magnitude – on the free faces $x = 0$ and $x = 1$: because there is no bonded surrounding any more; on the loaded faces: because expansion in x is prevented by condition (a), but it increases towards the center. The direction of relaxation is towards the center for T_1, and towards the free margins for T_2. Thus the two boundary conditions are opposite in effect and sign (Fig.23, arrows in fourth ring for conditions 1 and 2). They need to be modelled separately.

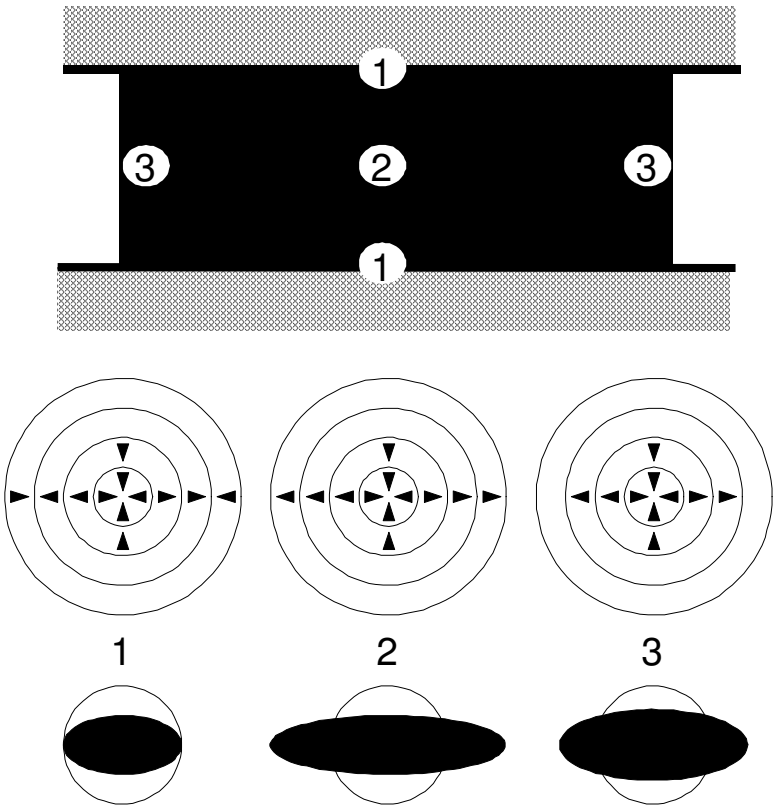

Fig. 23. Top: rectangular body of solid between two pistons with locations for the boundary conditions shown below. Center: boundary conditions as a function of location in the body. Circles symbolize (from center outward): operative force field (isotropic); normal component of deviatoric force field; dilational effect contributed by the system shear T_1; volume effect due to external boundary condition. The latter is directed inward in (1) due to the friction effect on the sample-piston interface, outward in (2) due to dilational effect supplied by the surrounding shear T_2, and zero in (3) for points on the interface between solid and freespace. Bottom: characterization of expected effect; white circle: unloaded state, black: loaded state.

12.2 The setup

In the static loaded state, system and surrounding do work on one another, but we cannot measure it; in thermodynamics only the work done in a change of state can be measured. No time-dependent processes are observed, system and surrounding are in equilibrium with one another, all fluxes are balanced. The quantity under investigation $T = T_1 + T_2$ is the work done by shear forces, a scalar quantity, resulting in a volume change, also a scalar quantity. It is thus possible to approach the modelling of the static state through a Laplace equation.

T_1 will be dealt with first. The distribution of a scalar quantity t_1 over a region $x(0 \rightarrow b)$ $y(0 \rightarrow d)$ with a maximum $t_1 = M$ for all points $y = 0$, and $t_1 = 0$ for all points $x =$

0, $x = b$, and $y = d$ is

$$t_1 = -4M\sum_{n=1}^{\infty}\frac{\sinh\left(\frac{m\pi(d-y)}{b}\right)\sin\frac{m\pi x}{b}}{m\pi\sinh\frac{dm\pi}{b}} \tag{52}$$

(Ref.13, p.546, eqn.2.17) where M is a magnitude scaling factor, b is the width of the solid along x, d is its length along y, and $m = 2\,n - 1$ (m is always odd). The reverse case is that of $t_2 = M$ for all points $y = d$, and $M = 0$ for all points $x = 0$, $x = b$, and $y = 0$,

$$t_2 = -4M\sum_{n=1}^{\infty}\frac{\sinh\left(\frac{m\pi y}{b}\right)\sin\frac{m\pi x}{b}}{m\pi\sinh\frac{dm\pi}{b}} \tag{53}$$

The combined effect is $T_1 = t_1 + t_2$. Along $x = b/2$ T_1 forms an upward-warping curve with a minimum $T_1 = -M$ for $y = 0$ and $y = d$, and a maximum ($M<0$) for $y = d/2$. Along $y = d/2$ T_1 forms a downward-warping curve with a maximum $T_1 = 0$ for $x = 0$ and $x = b$, and a minimum at $y = d/2$ (which is the maximum point on $x = b/2$).

For T_2 the boundary conditions are: $M = 0$ for all points $x = 0$, $x = b$, $y = 0$, and $y = d$, and increasing towards the center. This is done through

$$T_2 = b\sin\frac{\pi x}{b}\,d\sin\frac{\pi y}{d} \tag{54}$$

The sum $T = T_1 + T_2$ is interpreted as the potential for dilational cracking (Fig.24-27, upper panels). Of special interest is to find out were the gradients of T are the largest. Thus

$$\frac{\partial T_1}{\partial x} = -4M\sum_{n=1}^{\infty}\frac{\left(\sinh\frac{m\pi(d-y)}{b}+\sinh\frac{m\pi y}{b}\right)\cos\left(\frac{m\pi x}{b}\right)}{b\sinh\frac{dm\pi}{b}} \tag{55}$$

and

$$\frac{\partial T_2}{\partial x} = \pi\cos\frac{\pi x}{b}\quad d\sin\frac{\pi y}{d}\,; \tag{56}$$

the magnitude of the gradient is given by

$$\frac{\partial^2 T_1}{\partial x^2} = 4M\sum_{n=1}^{\infty}\frac{\left(\sinh\frac{m\pi(d-y)}{b}+\sinh\frac{m\pi y}{b}\right)m\pi\sin\frac{m\pi x}{b}}{b^2\sinh\frac{dm\pi}{b}} \tag{57}$$

and

$$\frac{\partial^2 T_2}{\partial x^2} = -\frac{\pi^2\sin\frac{\pi x}{b}\,d\sin\frac{\pi y}{d}}{b} \tag{58}$$

The derivative $\partial^2 T/\partial x^2$ (the sum of eqns.57 and 58) of the surface $T(b,d)$ is interpreted as the potential for shear cracking (Fig.24-27, lower panels). The derivative $\partial^2 T/\partial y^2$ gives identical results in the sense that the morphologies of both derivatives are identical, but

their absolute magnitudes are a function of the chosen absolute dimensions of b and d, respectively. For realistic results the model needs to be rescaled to real material properties.

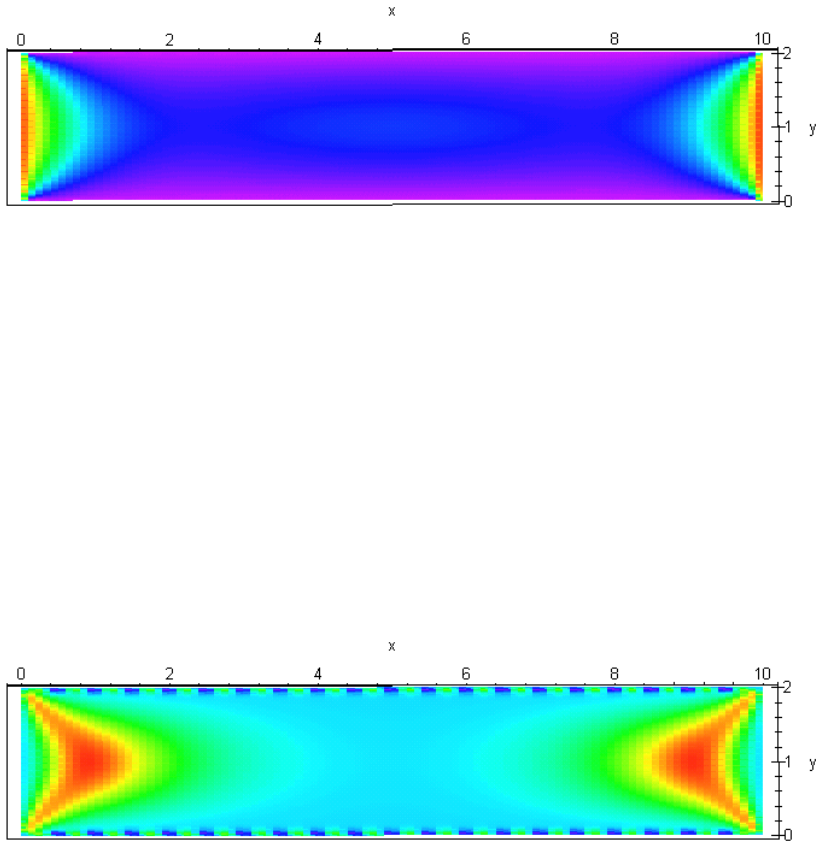

Fig. 24. Dimensions 10×2 distance units. Wavy structures along horizontal margins in lower panel are mathematical artefacts due to summing over non-infinite coefficients n.

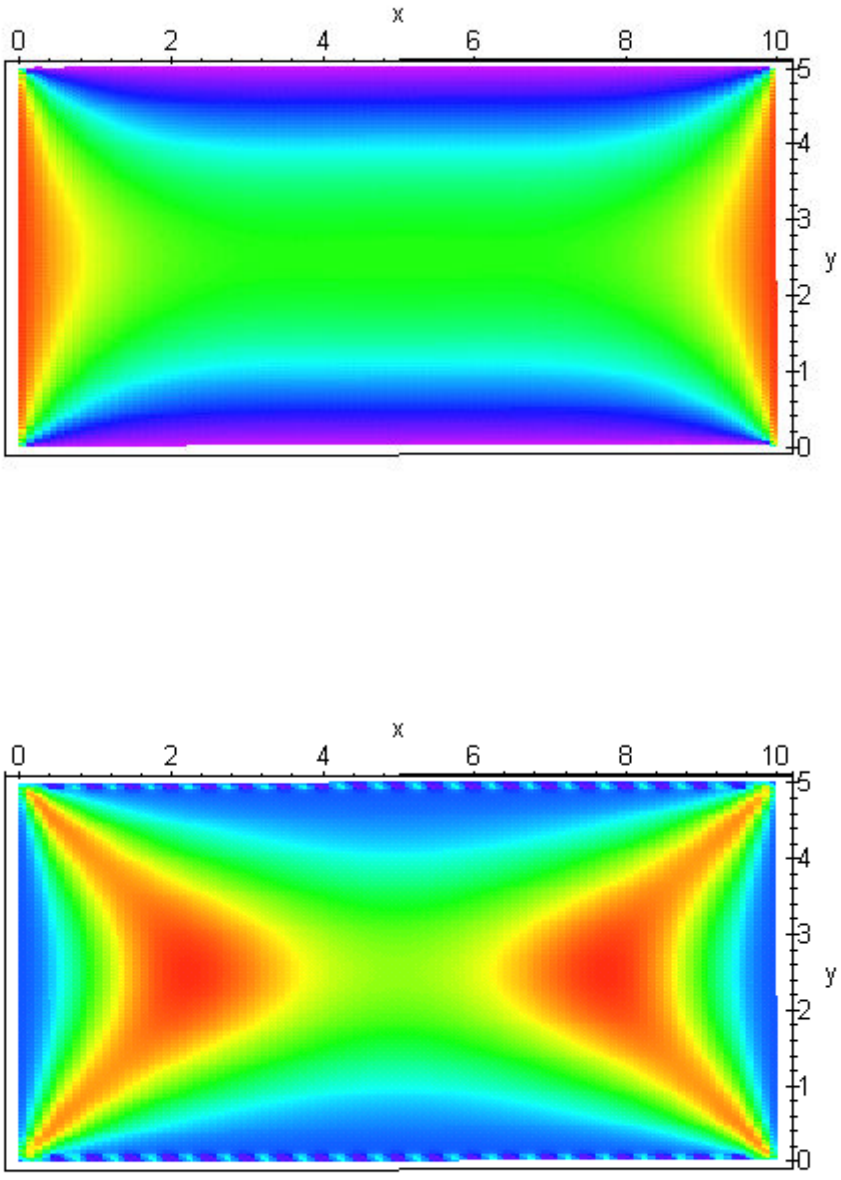

Fig. 25. Dimensions 10×5 distance units. Wavy structures along horizontal margins in lower panel are mathematical artefacts due to summing over non-infinite coefficients *n*.

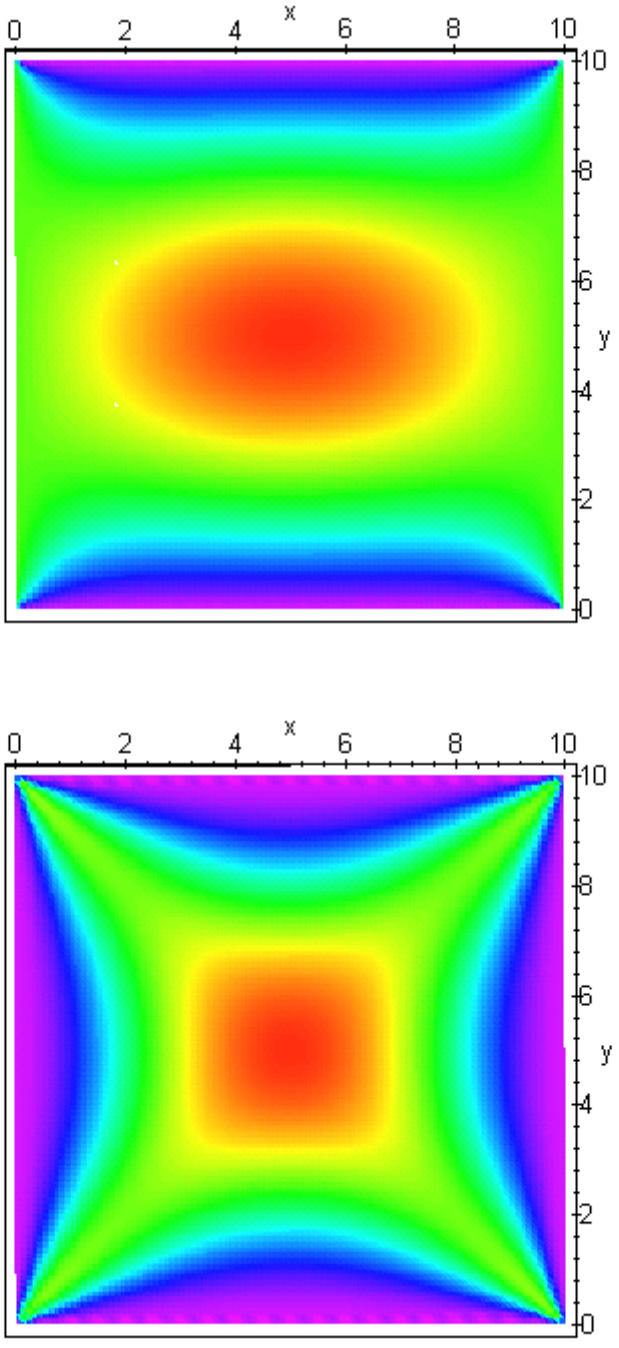

Fig. 26. Dimensions 10×10 distance units.

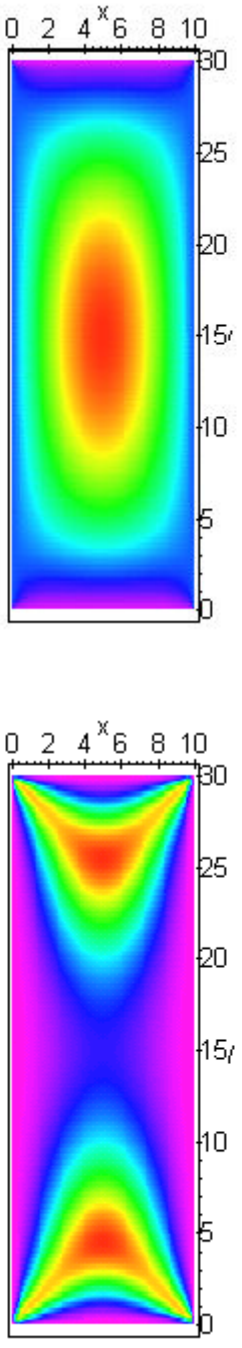

Fig. 27. Dimensions 10×30 distance units.

12.3 Results

The setup delivers all properties of the loaded state as a function of location within the region of validity *bd*. In a similar way it should be possible to derive the displacements by using the work function, and to calculate the shape of the deformed body.

In Figures 24-27, the upper panels show the potential for dilational cracking T, the lower panels show the potential for shear cracking $\partial^2 T/\partial x^2$. The width of 10 distance units is the same in all figures. Colors indicate relative magnitudes (purple = minimum, red = maximum).

For thick, short columns (Fig.24, height 2 units) the center is dynamically dead, it is under strong compression. The dilational crack potential is very close to the free surface, suggesting that a brittle material loaded to the elastic limit might spallate. The shear crack potential is farther inside the body, further destabilizing the surface, and low in the center. The failure potential distribution is strongly controlled by the zero-glide boundary condition along the loaded faces.

If the height of the body is only slighty increased (Fig.25, height 5 units), the dilational crack potential is still close to the surface, but the shear crack potential shifts very quickly into the interior of the body. The dilational and shear maxima no longer coincide.

In a body of square shape (Fig.26, height 10 units) the dilational crack potential and the shear crack potential again coincide, but this time in the center of the body, suggesting that any material yield, brittle or plastic, should start there.

Turning to a long, slender column (Fig.27, height 30 units) the dilational crack potential stays in the center of the body, but it extends along the long axis, decreasing only close to the loaded faces. The potential for shear cracking has left the center and shifted towards the loaded faces, it forms two maxima which peter out towards the center of the body, but they form sharp bifurcating extensions towards the corners of the body where the loaded and unloaded faces define a discontinuity in the boundary conditions. The two extensions and the loaded body surface form a triangular region which is also under low dilational effect; this triangle is largely dead. The calculations permit the interpretation that brittle yielding should start through dilational cracking in the center of the body; the cracks should propagate along the long axis (which will ultimately change the boundary conditions) up to the region where the dilational potential abates; but here the shear potential reaches its maximum, so the mode of yield should switch from dilational to shear cracking and propagate towards the corners. The material response predicted here is indeed observed in experiments on brittle materials such as ceramics.[47]

It is shown that the new approach to deformation theory can be used to model the loading conditions in a discrete body subjected to a specific loading configuration. In comparison to the theoretical approach used up to this date, the requirements on hardware and mathematical effort for the results presented here are nearly nil. The advantage in using a proper field theory is also evident as no grid of nodes is necessary, and a solution can be readily calculated for any desired point within the region of validity, using mathematical methods which have been long worked out for problems in other field theories. The results of the predictions also appear to be in close harmony with

observations as they are known to this author.

13. Discussion

The approach presented here is entirely free of Eulerian concepts. It observes the rules of potential theory and is merely a generalization of standard thermodynamics: whereas this theory is commonly taught as a scalar theory, implying isotropic external and internal conditions, this one permits to consider internal and external anisotropic boundary conditions. It turns out that its earliest conceptual roots can be traced back to the founding fathers of thermodynamics in the 19^{th} and early 20^{th} century. Hence the conceptual disparity between the Euler-Cauchy theory and standard thermodynamics has been open for everyone to see for 130 years, since the days of Clausius and Gibbs.

One single phenomenological argument was used – the Birch-Murnaghan equation – in lieu of the unknown solution to a quantum-mechanic problem, and I feel justified to do so as this equation is widely used, and known to yield satisfying results. Apart from that, no material constants were introduced. Their rightful place should be in the two field property tensors (eqn.4), and only there. The similarity of prediction and observation is rather good, at least in my eyes. The theory not only correctly predicts the fabric properties, but also the progressive kinematics of simple shear, such as the rotation of Riedel planes against the sense of bulk shear and against the sense of shear on the Riedel plane itself. It permits the conclusion that crystals in a glide position must also rotate at the same time, whereas crystals in a non-rotating position must be locked. The commonly held concept that crystal glide planes in simple shear zones align with the bulk shear plane such that the maxima are formed by non-rotating, yet actively gliding crystals, is therefore challenged at least for plastic deformation without recovery processes. The argument is supported by the observation that crystals in a maximum glide position must have the highest rate of lattice defect production; they should therefore be most likely to undergo recrystallization, they should be least stable, and they are least likely to populate the maxima.

The approach presents a straightforward one-to-one relation of force field to displacement field, both of which are vector fields controlled by tensors; from a mathematical point of view it is therefore more systematic than the Euler-Cauchy approach which claims a tensor to be the cause of the displacement vector field. It is also predictive, contrary to the Euler-Cauchy theory which does not permit the deduction of a particular displacement field from a known state of stress. Specifically, it avoids the unsatisfying conclusion that an orthorhombic state of stress can cause a monoclinic displacement field. It gives an explanation as to why mineral phases in shear zones are commonly much better equilibrated than outside; kinematically, it liberates the thinking from the symmetry constraints of Cauchy´s theory which must appear unrealistic to anyone familiar with simple shear. I am not yet aware of an observed aspect of material behavior that could be interpreted to be incompatible with this approach. On the contrary, this theory was developed in response to too many systematic questions left unanswered by instructors and text books, and in the course of its development it offered an answer to

nearly all of them. Still: although in most cases it was possible to follow the logic of a line of thought, there are certain details especially in the theory of simple shear where I found myself in completely uncharted waters. In order to proceed I had to make a decision and give preference to one alternative over another without being all too sure whether I am doing the right thing; and although the predictions appear to be satisfactory I remain sceptical. But it is better to go on and be wrong in some cases rather than do nothing out of fear of making a mistake. Much of this essay here I understand as a proposition in need of discussion.

Acknowledgments

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