Strain and displacement: energetic patterns in elastic and plastic deformation

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Abstract

The precise details of elastic deformation are more complex than is evident from the common theory of elasticity. Experiments show that elastic simple shear requires more work than pure shear, indicating that strain is not a thermodynamic state function. The natural alternative is displacement. A new approach to elasticity and deformation, a generalized thermodynamic theory for bonded materials, correctly predicts the simple/pure shear energetic difference. Experiments in the plastic realm show that simple shear costs substantially less work than pure shear, which is also predicted by the new approach.

Introduction

A recent review of conventional continuum mechanics revealed major conceptual idiosyncrasies in this theory. The First Law of thermodynamics is the energy conservation law of non-conservative physics, of exchange of energy between system and surrounding. In continuum mechanics it is given in a form which subordinates it to the conservative energy conservation law of Newtonian mechanics (Koenemann 2008a). This turns the First Law upside-down, it negates its very nature.

A *conservative* process observes $E_{kin} + E_{pot} = U = const$. It is thus a process that takes place *within* a system which exchanges neither mass nor energy with a surrounding. A *non-conservative* process is a process beyond and outside this law such that U is a variable. The properties of the system are considered per unit mass, and any energetic changes then come about through exchange of energy between system and surrounding. The energy conservation law for such a *non-conservative* process is thus $dU = dw + dq$. It may then be *reversible* $dq/T = 0$ or *irreversible* $dq/T > 0$. Elasticity is therefore by nature a reversible change of state in the sense of the First Law of thermodynamics: external work is done upon the system, and a potential builds up in the system which causes its reconstitution upon release. But the understanding of the loaded state in conventional continuum mechanics, commonly called stress σ, is based on Newtonian mechanics to this day (Koenemann 2001, 2008a). It is therefore conservative, and pre-thermodynamic; it cannot describe an energetic change of state of a system. For any process by which work is done upon a system V, the divergence of the acting forces must be non-zero,

$$\nabla\cdot\mathbf{f} = \varphi \neq 0; \tag{1}$$

this is the Poisson condition (φ = charge; Kellogg 1929). However, the Cauchy theory of stress σ leads to the commonly known condition that for a volume-neutral elastic deformation the trace tr $\sigma = 0$. This is a form of the Laplace condition

$$\nabla\cdot\mathbf{f} = 0, \tag{2}$$

which is one way of stating that no net work is done upon the system. Any theory of deformation that implicitly refers to eqn.2 instead of eqn.1 must therefore be invalid by definition. Kellogg (1929) discusses the Laplace condition in a chapter on "potentials at points of freespace", and the Poisson condition in a chapter on "potentials at points occupied by masses", such as the interior of a solid. The Laplace condition is equivalent to $E_{kin} + E_{pot} = U = const$ since U is invariant, a change of state is therefore ruled out. If the energy of a system is changed, U is necessarily a variable, and $\varphi \neq 0$ in the loaded state; any changes are then considered under $dU = dw + dq$.

There are certainly numerous texts which make attempt to combine the Cauchy stress theory with thermodynamic theory. However, this does neither correct the pre-thermodynamic mathematical structure of the former, nor its inevitable consequence, the zero work condition for an isochoric deformation (Koenemann 2008a). If a body is internally bonded, its internal pressure $(dU/dV)_T \neq 0$. This term has no place in Newtonian mechanics. In solids the internal pressure is in the order of several 100 MPa. The term *stress* is therefore avoided here in favour of the *loaded state*. An approach to elasticity which treats elastic deformation as a change of state, which builds up upon an equation of state and the First Law, and which arrives at a non-zero work result for a volume-constant elastic deformation, has been given by Koenemann (2008b).

In this paper theoretical predictions and experimental evidence shall be compared for both elastic and plastic deformation. Experiments have shown that elastic simple shear deformation requires more energy than elastic pure shear deformation per chosen strain ε, whereas plastic simple shear requires substantially less work than plastic pure shear, again per unit strain ε. There is thus an energetic inversion across the reversible-irreversible boundary. Its significance for the generation of geological structures has not been appreciated so far; and this author is not aware of an attempt to explain these energetic differences in a coherent way that applies to both sides of the elastic-plastic transition.

Elastic deformation work

Theoretical considerations

The work equation in physics is always the product of an intensive and an extensive term, the latter is the distance between a starting and an end point, or a path. Strain ε has so far been taken as a measure of deformation, so it seemed natural to consider it as a state function, in analogy to the thermodynamic PdV. However, the latter expression is isotropic. For anisotropic changes of state it needs to be generalized.

A state function is a physical parameter of a system of mass which only depends on its state in equilibrium. It is path-independent, or history-independent, and a function of the initial and final state only (Moore 1972, Atkins 1990), such as temperature, pressure, volume, internal energy, entropy. Mathematically, they are all scalars. The intensive terms are isotropic by definition. The spatial properties of the extensive terms have not been a matter of discussion as far as this author is informed. They certainly can be subject to boundary conditions; however, since thermodynamics was developed for equilibrium processes in a gas at rest, the boundary conditions are assumed to be isotropic by default, and correctly so: the surface-volume relation for a given mass is shape-dependent, but has an minimum value for a sphere; and it is impossible to find an average value for an intensity term (e.g. mole fraction) as a function of location in a heterogeneous environment if the shape of the thermodynamic system is unconstrained. In addition, gases do not have directional properties. The shape of the thermodynamic system is thus safely assumed to be of spherical shape unless better information is available. In solids this may well be the case, because they can be anisotropic.

The First Law is sometimes given in the ostensibly thermodynamics-compatible form

$$dU = -\sigma d\varepsilon - PdV + TdS \tag{3}$$

where the first term RHS contains the anisotropic part and the second term the isotropic part of the work term. Here, strain ε is used as a state function. However, in 30 years of literature research this author has not found a derivation or justification, not even the attempt at discussion. It needs to be emphasized that for a volume-neutral deformation both σ_{ii} and ε_{ii} are zero; $\sigma d\varepsilon$ therefore satisfies the Laplace condition (eqn.2), it is energetically empty (Koenemann 2008a). The question is if the use of strain as a state function is indeed correct. The natural alternative would be displacement.

Historically, the concept of strain is much older than thermodynamics. Cauchy (1827a) defined it in analogy to his stress theory (Cauchy 1827b). But only his strain theory can be related to Euclidean space, not his stress theory (Koenemann 2001). In effect, Cauchy's two theories cannot be related to one another. This may be surprising at first, but shows the great age of Cauchy's work which was done 30-40 years before the properties of vector spaces and the systematic foundation of linear algebra was worked out, without which it is not possible to generate a mathematically coherent spatial theory. It was also 40 years before the physics of the interaction of system and surrounding, i.e. the basics of thermodynamics, were sufficiently understood to serve as a model. It is not possible to deduce a proper cause-effect relation from Cauchy's theory; the latter is not satisfying for a modern reader because he set the torque to zero by default. But the torque integrated over all directions in space cannot be assumed to be zero without (a) a careful evaluation of the configuration of the acting forces as a function of the external boundary conditions, (b) the shape of the volume element upon which they act, and (c) the condition that system and surrounding are solidly bonded to one another. However, bonds were never considered in continuum mechanics, from Cauchy (1827b) to the 20th century standard text books (Truesdell & Toupin 1960, Gurtin 1981, Holzapfel 2000). Cauchy's interest in deformation was driven by mathematics. He was evidently fascinated by the representation of a quadric by an elliptical or hyperbolic plane, he mentioned it in his earliest note on this subject in 1821 already. It appears that he knew about this concept early on and turned to deformation to find an application for it – intuitively, and carried by his intellectual excitement. But there he jumped to conclusions. Cauchy's assertion – that rotational equilibrium exists, without argument – resulted in an unrecognized boundary condition, applying to uniaxial compression or plane pure shear only. His approach lacks generality. Simple shear deformation is the critical deformation type to test his theory. For more discussion see Koenemann (2008a).

For a modern understanding of deformation the thermodynamic theory offers excellent guidance. It starts with an equation of state; thereby the material properties are introduced. It distinguishes system and surrounding, which is not done in continuum mechanics. The system contains a finite mass – in mol, not in [kg] – which is the reference mass for the thermodynamic potentials. The external loading – a pressure increase in standard thermodynamics – gives the constraints, upon which the effect of the loading is calculated by means of the work equation PdV, so that the effect ΔV is a function of the material properties and the external boundary conditions exclusively. Thermodynamics thus has a clear order: material properties plus cause deliver the effect; the latter does not require a theory of its own. This conceptual framework was obeyed in the development of the theory outlined below (Koenemann 2008b).

Strain and displacement differ in their geometric and mathematical properties. Strain is an orthogonal tensor, and insensitive to constraints with lower than orthogonal symmetry. The strain ellipsoid rotates in a progressive simple shear, but it records only the relative stretch without reference to a coordinate system, and thus without relation to the boundary conditions. Instead, displacement is a vector field which may or may not be orthogonal, and which contains much more information than strain. Displacement thus appears to be the term to which a proper physical cause-effect relation should lead. The strain may then be derived from it, but not the other way round.

The study of deformation is strongly oriented towards strain because it appears natural to correlate two tensor quantities. However, since the current theory of stress cannot be correct – it is incompatible with potential theory (Koenemann 2008a) – that obstacle is removed. Workers studying simple shear have been trained to accept that the principal axes of finite strain rotate with progressive deformation. Principal axes are found through an eigenvector routine. But eigendirections cannot rotate in engineering mathematics, they are those directions in which only radial components exist. Rotating eigendirections are a clear sign that deformation as a theoretical problem is not properly understood; and the fact that the principal axes of both instantaneous and finite strain are not fabric-forming shows that they are indeed physically irrelevant. Koenemann (2008b) derived a displacement field for simple shear with stable, non-orthogonal eigendirections which are fabric-forming.

Experimental evidence

Boundary conditions always exist, and must be considered for any physical process; and the condition of path independence applies to the *energetic* state only, i.e. the deformation work. An elastic deformation is path-independent if it is reversible. If it is possible to subject a material to any deformation history D_1, … with free choice of strain magnitudes and boundary conditions, finally to end at some chosen set of external conditions D_{final} (boundary conditions and strain magnitude), the displacement is path-independent if the system is then always in the identical energetic state U_{final} independend ot the histories D_1, …, that is, if U_{final} is always the same under the conditions of D_{final}. On the other hand, strain can be a state function only if all identical states of strain $\varepsilon_{\mathrm{final}}$ cost the same amount of deformation work, independent of the boundary conditions.

Treloar (1975) performed experiments to map the energetics of elastic deformation of rubber as a function of the boundary conditions. He found that simple shear consistently requires 7-10% more work per unit strain than pure shear (Fig.1 left). Strain ε is therefore not a measure of the elastic work done in a deformation. It follows that strain is not a thermodynamic state function, whereas displacement is a state function. The boundary conditions clearly have a strong influence on the energetics of elastic deformation, but they have no bearing on whether an elastic deformation is path-independent or not.

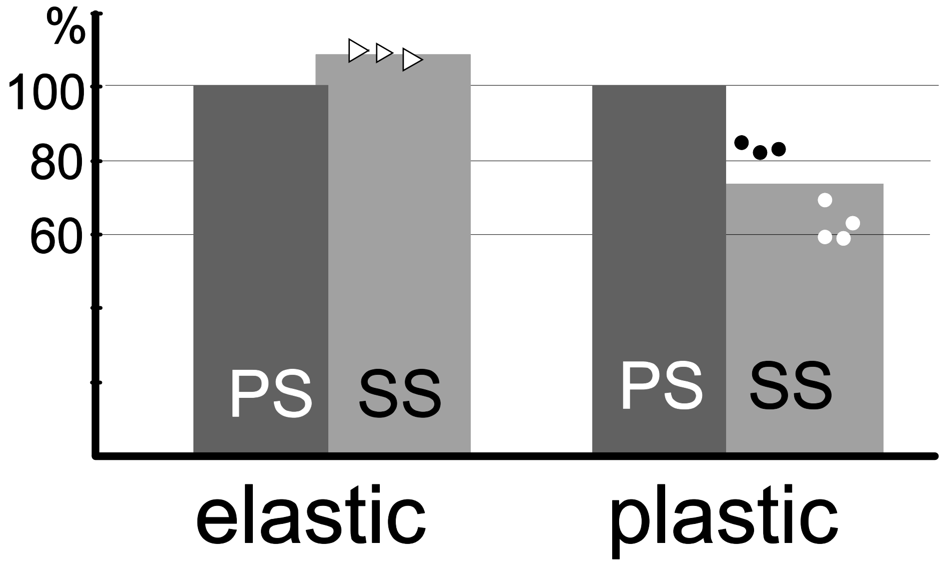

Fig.1 Energetics of simple shear relative to other deformation types. Columns: theoretical predictions (Koenemann, 2008b); elastic simple shear (SS) is expected to require 8,4% more work than pure shear (PS = 100%), plastic simple shear should require 26.7% less work than the respective pure shear. Triangles: Treloar (1975) PS and SS, rubber; black dots: Tome et al. (1984), copper, compression and torsion at 20℃; white dots: Franss en (1996), salt, compression and SS at 300 and 350℃.

The new approach: structure and predictions

The new approach (Koenemann 2008b) proceeds in a very different way. It is assumed that an elastic deformation is a change of state such that work is done upon a system, and vice versa. The approach therefore starts with the First Law and an equation of state. The external loading conditions and the material properties are mutually independent, but they both influence the resulting loading state. It is assumed that the system has a potential proportional to its mass which is in its zero potential state when unloaded. Furthermore, system and surrounding are thought to be solidly bonded to one another. This condition ascertains that equilibrium always exists. Then two vector fields are derived; the internal vector field represents the material properties (strength, anisotropy), it is the force field exerted by the system at the surrounding; the external vector field is exerted by the surrounding upon the system, its properties are controlled by the boundary conditions (pure or simple shear etc.). The loaded state is then represented by a third force vector field which combines the properties of the first two ones. The systematics is explained below, using a plane pure shear with eigendirections parallel to the coordinates X_i – maximum compressive loading along X_2, and minimum compressive loading along X_1. The coordinate origin Q coincides with the center of mass of the thermodynamic system. The material properties are assumed to be isotropic, the system surface forms a sphere about Q. The system is embedded in a bonded surrounding of infinite extent.

To calculate the deformation at a point Q with given internal and external conditions, it is assumed that the ideal deformation state is the one that requires a maximum of work, which is an isotropic volume contraction. It is thereby assumed that any deformation implies an isotropic, inward-directed force field which is called the *operative force field* $\mathbf{f}_{op}$; it represents the average loading and is always non-zero. (This assumption makes the new approach different from the older ones, it observes the Poisson condition eqn.1.) The *deviatoric force field* $\mathbf{f}_{dev}$ is then constructed such that its average over all directions is zero relative to the ideal change of state. The deviatoric field is then further decomposed into a *normal force component field* – force components $\mathbf{f}_{dev\_n}$ colinear with the radius – and a *shear force component field* – force components $\mathbf{f}_{s(syst)}$ perpendicular to the radius. (1) The field $\mathbf{f}_{op}$ causes the system to contract isotropically. *PdV*-work is done upon the system. (2) The field $\mathbf{f}_{dev\_n}$ causes the system to contract along X_2, and to expand along X_1, such that the shape changes; the operation is volume-neutral, and no net work is done. (3) The field $\mathbf{f}_{s(syst)}$ represents the shear component exerted by the system at the surrounding because the system dilates by itself in X_1 due to the law of least work. The system therefore exerts shear forces at the surrounding. The effect of this step is an energetic relaxation to the energetic equilibrium state if the system surface in X_1 were unbonded. (4) The field $\mathbf{f}_{s(surr)}$ represents the shear forces exerted by the surrounding upon the system. This step has the same effect as the system shear forces, the result is a further dilation along X_1, but the system is then under external tension in X_1.

All work done has a volume effect. Work done by shear forces has only one sign, irrespective of the sign of the torque, because the spatial effect of a shear force is always dilatory. The sum of the four components is the *effective force field*,

$$\mathbf{f}_{op} + \mathbf{f}_{dev\_n} + \mathbf{f}_{s(syst)} + \mathbf{f}_{s(surr)} = \mathbf{f}_{eff} \tag{4}$$

If the work equation is applied, the field $\mathbf{f}_{eff}$ yields the elastic *displacement field* such that force field and displacement field have identical properties, i.e. they both contain all the information required to define the energetic and geometric state of the system (Koenemann 2008b). The strain ε can then be extracted if desired. – The component $\mathbf{f}_{s(surr)}$ can be mechanically active only in a bonded continuum; it must be zero along solid-freespace interfaces. This will cause gradients in any discrete sample as a function of sample shape and loading configuration.

Model calculations for pure shear and simple shear for a system in an infinite bonded continuum indicate that the work done in elastic simple shear is ca. 8% higher than work done in pure shear (Fig.1 left). Thus the prediction of the new approach is in harmony with the observed experimental data, confirming that strain ε is not a thermodynamic state function. Instead, displacement is a state function, which becomes apparent if deformation types with non-orthogonal properties are considered.

Plastic deformation work

State functions cannot be the issue in a consideration of irreversible plastic deformation work because entropy production depends on mechanisms, time-dependent processes, and other parameters. Nonetheless, strain is not a measure of deformation work in plastic deformation either. Tome et al. (1984) conducted experiments with copper in axial compression and in torsion, and found that torsion costs ca. 18% less work than compression (Fig.1 right). Franssen & Spiers (1990) and Franssen (1996) conducted experiments with rock salt for axial and simple shear. Their difference between the work done in simple shear and compression is in the order of 38% (Fig.1 right). Tome et al (1984) sought to find an explanation for their results in the theory of plasticity. Franssen & Spiers (1990) put more weight on deformation mechanisms and transport processes in the crystal lattice. Both studies had to admit that a compelling reason for the energetic difference they discovered is wanting.

Koenemann (2008b) extended the new approach to the initiation of plastic deformation. At the yield point the deformation switches from reversible to irreversible; hence bonds are broken, the absolute magnitude of loading no longer rises, and the fields $\mathbf{f}_{op}$, $\mathbf{f}_{dev\_n}$, and $\mathbf{f}_{s(syst)}$ no longer require any work. All further work is then done by shear forces $\mathbf{f}_{s(surr)}$ only. This is only half of the shear work required for elastic deformation which is then dissipated energy. The approach predicts that a plastic simple shear deformation requires 26.7% less work than a plastic pure shear deformation for the same strain.

The theory says nothing about mechanisms of plastic flow, and reality surely is more complex than these simple models. Natural flow of rocks is known to be strongly rate-dependent, which has not been considered here. However, the predictions are in sign and magnitude comparable to the experimental results, even if they are not expected to be the last word in this matter.

Discussion

Deformation types are not energetically equivalent, neither in the elastic nor in the plastic realm, and naturally those that cost the least amount of work are favoured by nature. In the elastic realm this is the deformation type with the highest symmetry state, i.e. orthorhombic, or even axial. In the plastic realm it is simple shear.

Strain was devised by Cauchy (1827a) as a purely geometric device. It is a term that can be easily measured, thus it is certainly not without value in practical applications; but as an energetically relevant term strain suffers from the same deficiencies as Cauchy's theory in general. The early 19th century was not the right time yet to fully comprehend the physics of deformation. The error does not become instantly obvious in loading configurations with orthorhombic or higher symmetry properties because the deformation types with higher symmetry properties are favoured by nature in the elastic realm due to the law of least work (Fig.1). The critical deformation type to test the validity of strain as a physical parameter is therefore a deformation with less than orthogonal properties, but such experiments were not done before Poynting (1912) and the studies in the 1950s (cf. Treloar 1975).

Any deformation starts with elastic deformation. Its contribution to the total deformation may be insignificant in geological materials, but the elastically loaded state determines the force configuration in the loaded state. Thermodynamics, which is the physics of continua, has been a very successful theory for gases and fluids. The boundary condition in standard thermodynamics – e.g. in a pressure increase – is implicitly isotropic, so the theory is commonly and correctly given in scalar form. The new approach (Koenemann 2008b) is a reformulation of standard thermodynamic theory in vector field form, such that anisotropic material properties and anisotropic external boundary conditions can be considered. The predictions for the energetics of elastic and plastic deformation are supported by observations.

The conventional theory of elasticity is pre-thermodynamic in mathematical and physical structure, and the term it offers for the quantification of a deformation – strain – does not contain sufficient energetic information to be fully descriptive. The conventional theory usually assumes implicitly or explicitly that the volume of a system to be deformed remains constant (incompressibility). This is systematically questionable, it imposes an unnecessary boundary condition, and it ignores the Poynting effect, also called dilatancy, which causes a body subjected to elastic simple shear to dilate elastic-reversibly (Poynting 1912, Reiner 1958). Instead, the new approach (Koenemann 2008b) is sensitive to boundary conditions, it provides a clear cause-effect relation, it derives its mathematical structure from thermodynamics, it treats displacement as a state function, it correctly predicts the elevated work required in elastic simple shear relative to pure shear, and it predicts the Poynting effect.

The discussion on the generation of discrete shear zones in geology has centered on mechanisms. Poirier (1980) distinguished five: geometric softening through fabric alignment, structural softening through recrystallization and grain boundary migration, strain hardening through dislocation entanglement, strain rate softening, and thermal softening. The cause of shear localization has therefore been sought in the material and its changing properties as a function of deformation. Implied in all this is the assumption, so far unquestioned, that strain ε is a physically meaningful term which is directly associated with a given amount of work. However, this is not the case. Rather, the specific deformation type itself may be the cause of softening, independent of any material properties in particular, if the energetics of deformation are not the same for the various boundary conditions. On the contrary, if simple shear is so strongly energetically favoured in the plastic realm, the law of least work suggests that a homogeneous body should decay into narrow shear bands, with large regions in between which behave passively, and heterogeneous flow should be the overwhelming rule. This is not to say that other mechanisms originating in the material do not exist, they surely do; but a search for the mechanism of shear concentration misses the point if simple shear itself is the reason.

Elastic effects are commonly ignored in studies of plastic deformation. However, the positive energetic deviation of simple shear in relation to pure shear in the elastic realm may be directly linked to the negative deviation in the plastic realm. Since all shear causes dilation, the material can be said to be constitutionally expanded; sub-volumes subjected to simple shear boundary conditions within a bonded continuum may thus reach the yield point earlier, and plastic deformation may thus be initiated more easily. After all, both the experiments by Poynting (1912) and Tome et al. (1984) were done in torsion.

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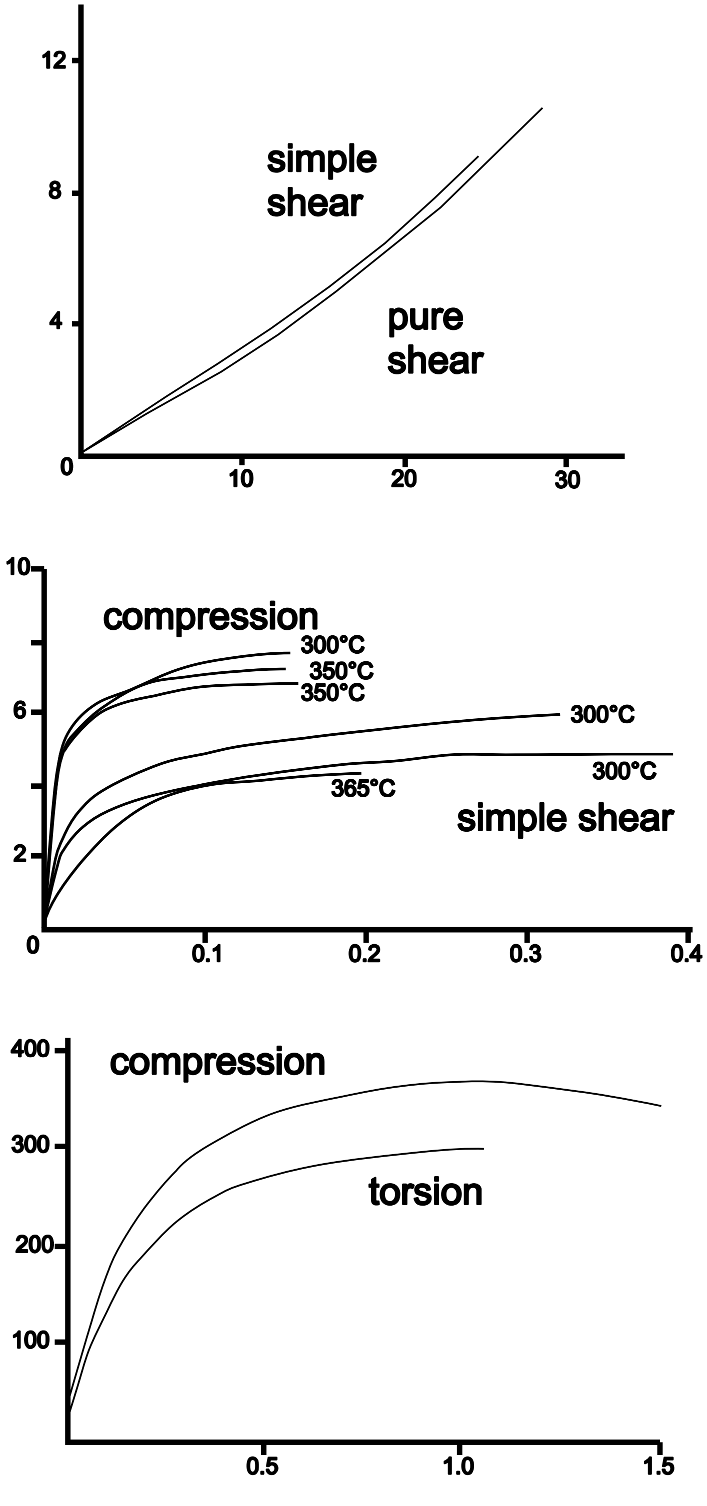
Supplementary Figure



Supplementary Figure. Experimental data (redrawn) for simple shear and pure shear or axial compression. Abscissa: strain, ordinate: pressure in MPa. Top: elastic deformation of rubber (Treloar 1975). Center: deformation of salt in compression and simple shear at the temperatures indicated (Franssen and Spiers 1990, Franssen 1996). Bottom: deformation of copper in torsion and compression at room temperature (Tome et al. 1984). The data points in Fig.1 above are readings from these data here.