

Deformation with Diffusion: the Growth of Augen

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Abstract: Stiff resistant inclusions in a deforming rock generate local stress concentrations and stress gradients. The resulting diffusive mass transfer is partly along grain interfaces and partly through grain interiors. For the latter effect, two different sets of fundamental ideas are in use. In either version, the effect of diffusion is to enhance strain rates and to moderate stress concentrations. In the first version, local diffusive loss is isotropic and can change an infinitesimal spherical element only to a smaller sphere whereas in the second, local diffusive loss can be anisotropic and can change a sphere to an ellipsoid.

The problem used as illustration is that of a highly viscous embedded cylinder in pure shear. Each version yields predictions of diminished stress concentrations and enhanced strain rates, and invites further development. The second version is favored; by extension, a material component's chemical potential at a point is seen as being like the normal stress at a point, i.e. multivalued, every planar element through the point having its own associated value.

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Editor's Note

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Introduction

Among the purposes of the present volume is that of recognizing Win Means's contributions to our science, and among his contributions is his emphasis on the "global classroom." The perpetual student, the teacher who is also an eager learner, has been with us since classical times; nowadays, with electronic help, geologists can converse regardless of distance; the classroom in which we learn from each other is global indeed. I think Win would agree that it is more a seminar room than a lecture hall: avoiding the dogmatic, a proper use of global facilities is to put forward exploratory ideas so as to prompt colleagues to work them over.

These prefatory remarks are supposed to excuse the fact that the following proposals are only incomplete and tentative. I would like to have been able to link all the threads and reach conclusions that were incontrovertible, but have not been able. Readers will please exercise their own insight, and honor Win by treating the classroom as one where progress is cooperative. I hope others will continue to pursue the threads here taken in hand.

Stresses as a topic of study by themselves are of only limited interest, and the same is true of strains; it is in the interplay, when a stress causes a strain, that the topics come alive.

The link between stresses and strains is the material's rheology. To get started in the simplest manner, one can imagine a Newtonian material, one whose viscosity remains the same no matter what stress magnitude develops. But the outcrop geologist is soon forced to note a defect of Newtonian models: they make no allowance for diffusive mass transfer, whereas outcrops are full of evidence of such effects; differentiated cleavage zones and the gap-fillings between boudins are just two from a long list of manifestations.

Diffusion effects were incorporated in abstract general formulations of mechanics in the 1960s, but the first results

for specified realistic geometries were produced by Green (1970, 1980) and by Fletcher (1982). Fletcher described diffusion in three situations:

- (i) across a homogeneous bar when bent;
- (ii) along an inhomogeneous bar when compressed across its width;
- (iii) in an almost-planar layer at the onset of folding.

The second situation was explored further by van der Molen (1985) and examined independently by Stephenson (1988). Except for Fletcher's problem (iii), all of these can be called "one-dimensional" examples: the materials are taken to fill space in three dimensions, but it is in only one direction that a gradient exists driving a diffusive flux. Computer-chip design has prompted more one-dimensional studies (e.g. Greer 1995; Daruka et al. 1996) but in the present work we seek an example to extend Fletcher's exploration in two and three dimensions.

Definitions: in subsequent paragraphs the following two effects are considered to be separate. Let a large sample be imagined as divided into many small elements; each element is defined by the atoms that sit in its boundary, as if one could, for example, paint them. In "deformation without diffusive mass transfer" or "deformation at constant volume," the elements all change their shape but no atom migrates out of one element across a boundary into another element; the material contents of each element do not change. By contrast, "diffusive mass transfer" here means the migration of a few atoms through the main mass of non-migrators, and includes the migration of a few atoms across boundaries. Time is considered divisible into small intervals, so that in any interval only a small fraction of the total atom population migrates or diffuses; the vast majority remain in a coherent mass, so that the element boundaries remain well defined, though in need of constant touching up. But averaged over time, all atoms behave alike; every atom spends most of its time being coherent with its neighbors and has only brief spasms of action as a diffuser. In subsequent paragraphs, "viscous deformation" and "creep" refer to the first process, to deformation with no change of element contents, and "diffusion" is used for only the second process, in place of the more cumbersome "diffusive mass transfer."

In other contexts, of course, one might distinguish creep that occurs "by diffusion" from creep that occurs for example by glide on glide-planes, while both are envisaged as processes at constant volume. It is for the present paper only that "diffusion" is used in the special sense noted.

A simple assembly with two-dimensional cross-section is shown in Figure 1. A cylindrical inclusion with high viscosity is embedded in an extensive matrix of less viscous material; at all points remote from the inclusion, the stress field is uniform --- a north-south compression $M+S$ and a smaller east-west compression $M-S$; the situation extends uniformly perpendicular to the plane of the diagram so that, for all particles in the plane of the diagram, their velocities lie in the plane of the diagram too. Regions of greater compression exist around X,X and regions of less compression exist around Y,Y ; if diffusive fluxes exist at all, they will carry material away from X and toward Y . In the simplest formulation, we assume that each of the materials, --- (i) the inclusion and (ii) the matrix, --- has a constant isotropic viscosity, a constant coefficient of self-diffusion and constant density. For materials that show no self-diffusion at all, equations were developed over a century ago that accurately describe the resulting instantaneous strain rates and velocity field, but for materials with self-diffusion, the behavior is still not properly known.

As far as I know, the most extensive study of this problem yet made is the one by Finley (1994, 1996). Kenkmann and Dresen (1998) cover many aspects but exclude diffusion. Ideally, one might specify material properties and then try to discover the stress field that would exist around the inclusion without any preconceptions. However, a powerful exploratory approach is to make some assumptions about the stress field and ask, "What material properties would allow a stress field of this particular form to exist?" Using this approach, Finley shows a suite of possible stress fields for different degrees of contrast between inclusion and matrix, but all depend on the material being anisotropic; not only anisotropic but anisotropic to just the right extent and with the right variation from point to point to allow the stress field to be of the form assumed. The results constitute a valuable first attack on the problem and are highly instructive, but they prompt the thought, "Let us approach this problem again with particular attention to the matter of isotropy. If we insist on the materials being isotropic or close to it, in what way does this guide us as regards possible stress fields? Can we progress on and describe stress states that could exist in materials with less pronounced anisotropy? (N.B. Fletcher, in this volume, considers the same geometry but treats only transport at the interface whereas Finley's work and the present paper treat transport through the body of the materials.)

Preview of conclusions

Regrettably, I think this problem has no elegant solution; stress fields such as Finley described, using a small number of intelligible terms, are perhaps not found in ideally isotropic materials; even this problem, selected to be the simplest possible that admits diffusion in two dimensions, perhaps suffers from intractable awkwardness. However, the second approach, emphasizing the material's isotropy, brings some points of interest to the fore. I will therefore run through them, and hope that someone using Finley's insights as well as the present points succeeds in making a fruitful attack on this resistant problem.

Aside from the matter of isotropy, two more features of the present work are:

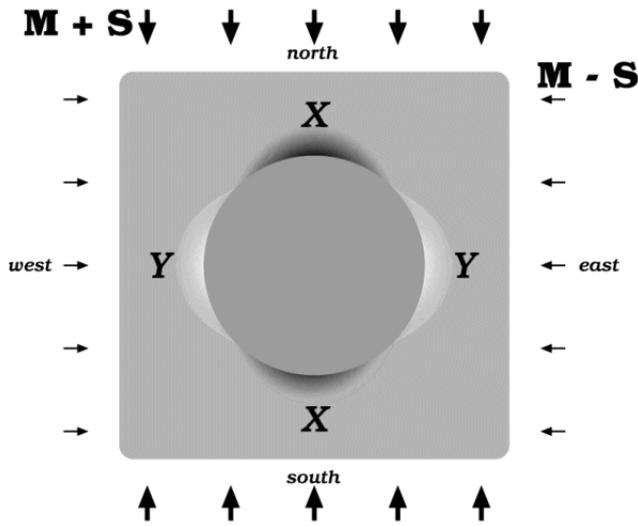
- (1) attention to the condition of plane strain, which is less simple in presence of diffusion than in its absence, and
- (2) attention to the possibility that when stress drives diffusion, the loss or gain in a material element may not be by the same amount in all directions: diffusive loss may turn a spherical element into a smaller ellipsoid, not necessarily a smaller sphere.

In fact, part of the purpose of the present piece is to bring the second idea forward and to explore it.

The classical solution extended

An intuitive picture of the stress state close to a stiff inclusion is shown by the shading in Figure 1. The quantity indicated is the mean stress, with two high-compression regions outside the inclusion to north and south and two regions of lower compression, "stress shadows," to east and west. The variation in mean stress is shown more quantitatively in Figure 2A; if, as shown in Figure 1, the remote stress field has principal stresses $M+S$ and $M-S$, then against a rigid inclusion in absence of diffusion, the extreme values of the local mean stress are $M+2S$ at the north and south interface points, and $M-2S$ at the east and west points (Muskhelishvili 1963; Jaeger and Cook 1979). The values diminish outwards in proportion with the square of the radius, so that at $r = 2R$, the anomalies are only one-quarter of their maximum values, and so on (r = radial coordinate; R = radius of the inclusion, hereafter taken as the unit length).

Figure 1. Cross-section of a long stiff cylindrical inclusion in a less stiff matrix.

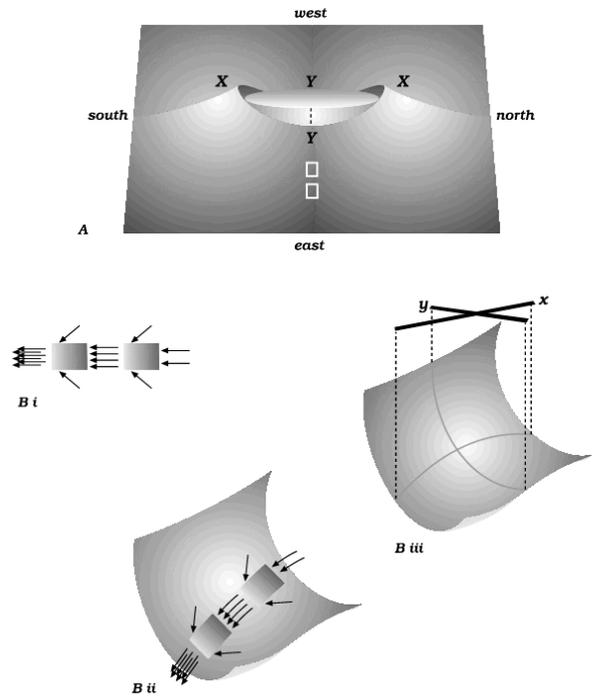


The matrix is assumed to extend without limit, and the uniform stresses shown are actually applied at a great distance from the inclusion. The shading shows locations of maximum and minimum compression.

Algebraic details are given in Appendix 1, but already an important point about the mean-stress surface can be noted. If diffusion were to start up but was sufficiently slight that the stress field was hardly modified, the gradients in Figure 2A could be thought of as the driving agents. Focussing, for example, on the east valley, we should expect diffusion into the valley from either side and also from its shallow upper end (the foreground of Figure 2A). But the valley-bottom descends more steeply close to the inclusion, and the variation specifically with radius to the power of two has the following property: if the diffusive flux is proportional to the mean-stress gradient, then over any section of the valley floor, the material diffusing out from the lower end exceeds what diffuses in at the top end by just enough to exactly balance the inflow at the sides; see Figure 2B (i) and (ii). The profile across the valley is concave upward but the profile along the valley is concave downward; if we write for the mean stress and use local axes x and y as in Figure 2B (iii), then

$$\frac{\partial^2 \bar{\sigma}}{\partial x^2} = - \frac{\partial^2 \bar{\sigma}}{\partial y^2}$$

Figure 2. A surface representing the mean-stress magnitude

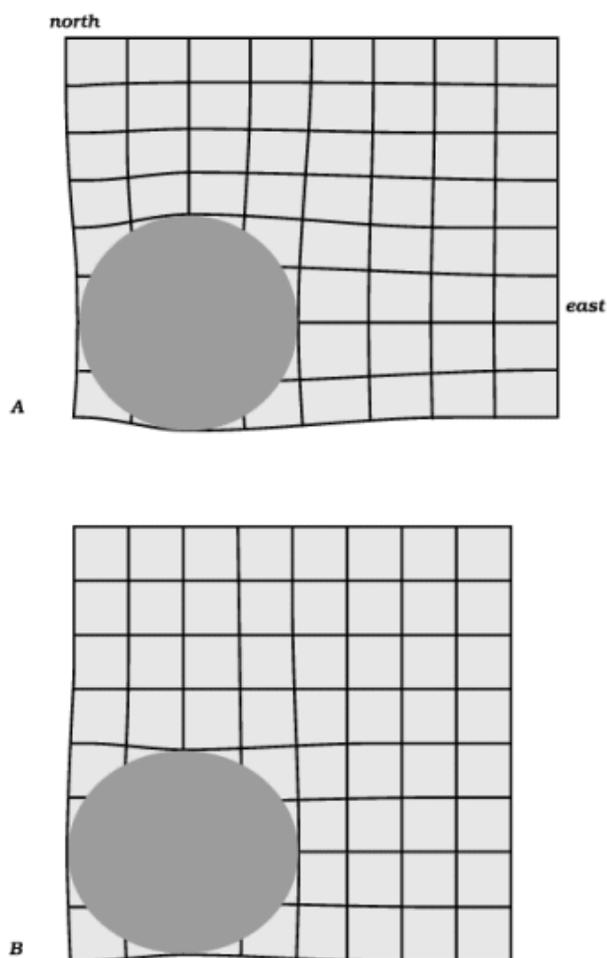


Shown here in the neighborhood of the inclusion; locations X,X and Y,Y are as in Figure 1. Far from the inclusion, the surface is flat at magnitude M . Part B of the figure shows details of the east valley.

The fact that this particular balance exists means that diffusion could indeed run without affecting the stress field. As so far described, the diffusion process would have no effect on the material's shape at any point. If we could just take care of effects at the interface, by finding a home for material that runs to the interface down the east and west valleys and supplying material so that it can run away from the interface at the north and south humps, we should have a system capable of running in a steady state.

To pursue this possibility, imagine that the cylindrical inclusion is stiff but not totally rigid. The pattern of mean stress would be changed only slightly, but the velocity field would change in an important respect: the cylinder's boundary would no longer be stationary but would become a changing ellipse in cross-section; if the cross-section were a circle at one moment, at later times it would become shorter north-south and longer east-west. An illustration of such a change is given in Figure 3.

Figure 3. Deformation of a grid that is initially composed of uniform squares.



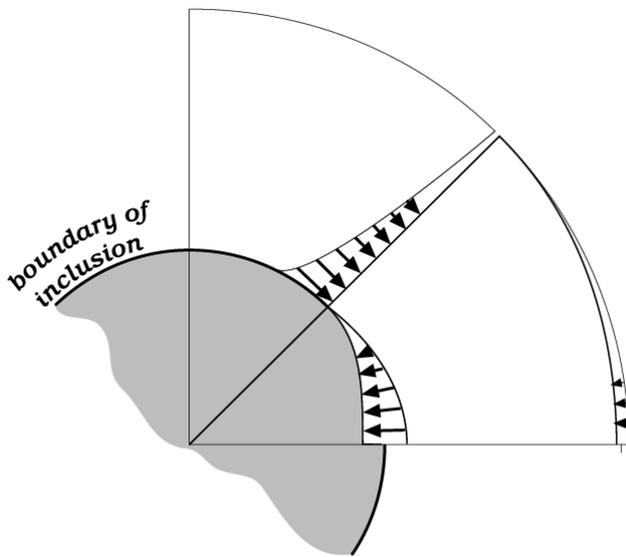
Part A shows how such a grid would change if the inclusion were rigid and the matrix was deformed. Part B shows how the grid would deform if the remote surroundings stayed still but the inclusion changed shape. We can assume that the inclusion is rigid, as in A; but in the surroundings, suppose that the change shown in B is superimposed on the change shown in A: then a gap would develop to east and west of the inclusion, and a conflict would exist to north and south, with inclusion and matrix both imagined to occupy the same space. Diffusive mass transfer could obviate the gap and the conflict.

The point now to be made is: if this velocity field were to exist in the inclusion's surroundings when the inclusion was in fact totally rigid, there would be a mass conflict at the north and south interface points (excess material to be got rid of) and a mass deficit at the east and west points (material would be needed to fill the gap). These are exactly the conditions that diffusion could take care of. In other words, if diffusion were to occur, the matrix could move as if the inclusion were deformable when in fact it was not;

or more generally, if the inclusion were slightly deformable, the matrix could move as if it were more readily deformable because of the easing effect of the diffusive fluxes.

The preceding ideas are quantified in Appendix 1, and illustrated in Figure 4. If stiff viscous materials were important in everyday engineering, the equations in Appendix 1 would have been worked out long ago; the reason that they or some equivalents have not been worked out before is partly that elastic behavior has commanded more attention, and partly that diffusion effects in everyday engineering occur on very short length scales. A conclusion from Appendix 1 is that for diffusion effects to be of consequence, the radius of a rigid inclusion needs to be only a few multiples of the material's characteristic length. (For comment on the idea of characteristic length, see Appendix 2). This means that in metal alloys we would need to be looking at resistant particles measured in nanometers, and in dry, hot creeping mineral aggregates we would need inclusions measured in micrometers (Bayly 1992, p. 120). By contrast, the purpose here is to contribute to the study of outcrops: we seek relations between stresses and strain rates that allow for diffusive mass transfer so as to understand augen, stylolites, saddle reefs etc., with dimensions in centimeters or meters. Fletcher (1982) has addressed this point and suggested that for a rock that self-diffuses by movement of dissolved quartz, the characteristic length might be of the order of 10 cm; but of course there remains considerable doubt about what behaviors in a wet granular rock resemble behaviors in an idealized continuum.

Figure 4. The intensity of the diffusive fluxes.



The tangential flux is greater close to the inclusion than farther out and is at a maximum across a plane at 45°, diminishing to zero on planes running due east or north. The radial flux similarly is strongest at the interface, but is zero at 45° and at a maximum along an east line (flux inward) or a north line (flux outward).

Defects in the description so far

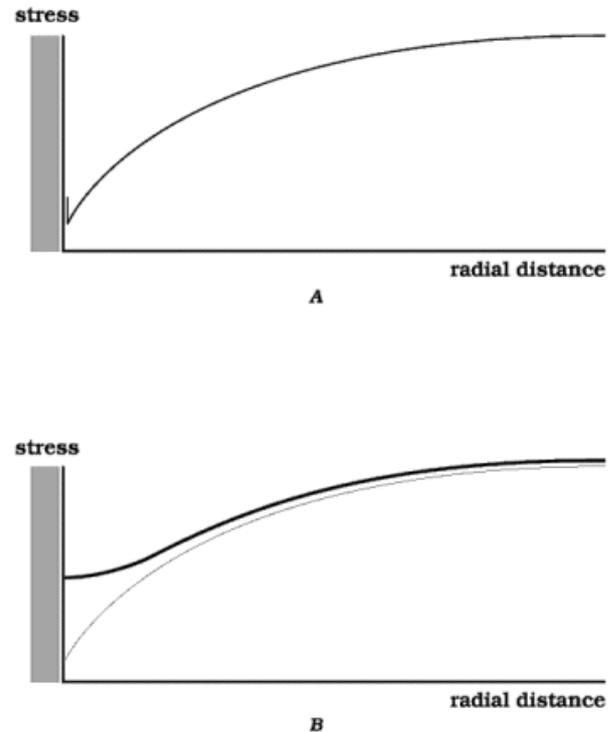
The description so far is defective in that:

(1) it describes only effects driven by the mean-stress magnitudes and gradients, --- no attention has yet been paid to σ_r and σ_q separately.

(2) it does not show any volume-element of material shrinking or expanding, --- losing or gaining material, --- by the diffusive mass transfer. The material that diffuses is deposited all in one location, at the interface, separate from the material it has diffused through. I would like to make the change illustrated in Figure 5, from the condition in part A to the condition in part B; that is, from the condition where deposition is strictly at the interface to a condition where deposition is distributed throughout a finite region of the host material.

The remainder of the text is an effort to circumvent these two defects.

Figure 5. Possible profiles of mean stress along the east valley.



Part A shows a profile as discussed in the text and shown obliquely in Figure 2. It is in two parts, a portion that is concave downward along its full length and a vertical portion or step at the interface (represented by the short vertical line just outside the interface). These two parts meet in a point that can be regarded as a concave-upward portion with infinite curvature and infinitesimal width. By contrast in part B, the portion that is concave upward is of finite width. A stress field with this type of profile leads to material accumulating by diffusion in a dispersed manner throughout a finite region of the host material, rather than in the localized manner of part A. It is this type of profile that is sought in the second half of the text. For part B, one can still assume that the north profile has the form of the east profile inverted, and that exactly the same distribution of material is lost from north and south regions as is gained by the east and west regions; those aspects of the problem remain simple.

Diffusive Gain or Loss not Isotropic

The present decade is interesting in that two different ideas about diffusive gain and loss are in use. Consider an extensive sample of material in which the stress is everywhere anisotropic and is also non-uniform. In particular consider a small spherical element somewhere within the

sample: if the material is viscous but non-diffusing the element will undergo strain at constant volume, but if it is self-diffusing as well as viscous, it will deform with principal strain rates that in general do not conserve volume. In principle, one could run parallel experiments and, by subtraction, isolate just the strain rates attributable to the diffusive process. Then the two ideas are:

(1) these isolated or partial strain rates must be the same in all directions (i. e. diffusion by itself can turn a sphere only into a smaller or larger sphere)

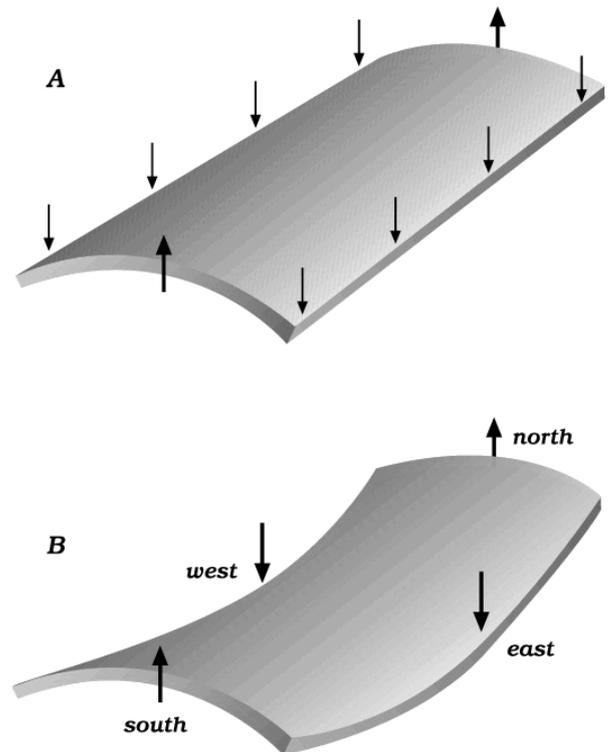
or

(2) the partial strain rates form a set whose principal values at any point are in general different from one another (i. e. diffusion by itself could turn a sphere into an ellipsoid).

In the first theory, to predict diffusive effects one looks at magnitudes and gradients of just the mean stress; in the second theory, one has to look at all three separate principal-stress magnitudes rather than just their mean.

For illustration, consider the bending experiments in Figure 6. Everyone agrees that in cylindrical bending, diagram A, diffusion can be initiated with a flux from the inner surface to the outer. But in saddle bending, diagram B, opinion is divided. In the center of the slab, the mean stress is uniform from top to bottom, but vertical planes running north-south are compressed more strongly normal to the plane in the lower part of the test slab than in the upper part, while vertical planes running east-west are compressed more strongly in the upper part; that is, there are gradients in the normal-stress components on these planes, that cancel each other out to give no gradient in mean stress. One wonders, Do the gradients drive diffusive fluxes that contribute to the deformation of the saddle? As far as I know, no such experiment has been reported. To imagine spherical atoms like billiard balls favors the idea of no diffusion in such a slab, but to imagine dislocation loops, incomplete atom-planes and dislocation climb favors the idea that the gradients could drive some loops to shrink and some to swell. I wish to give both ideas serious attention and respect, but in this section it is the second that we explore.

Figure 6. Two possible bending experiments



Two possible bending experiments where diffusive transport in a vertical direction might occur.

[Idea 3: if the material itself is anisotropic, --- for example, having a microstructure that is flaky or fibrous --- loss by diffusion may be greater in one direction than in another for that reason. But this idea is wholly separate: in the present paper, the material itself has no anisotropy, it is from the stress state that the anisotropy of the strain rates arises.

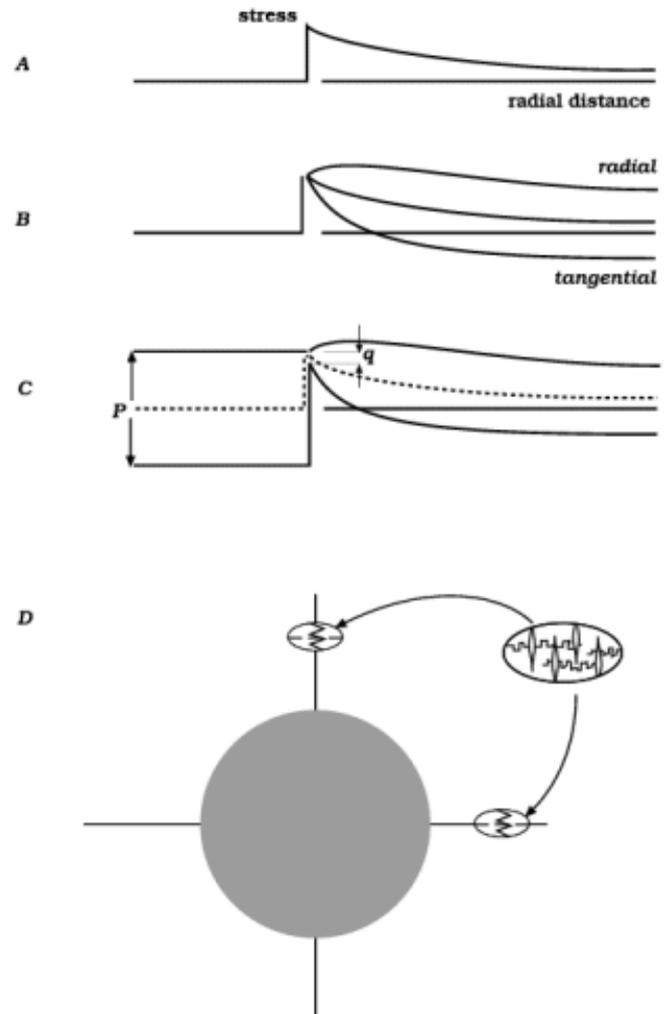
For a fourth idea, concerning gain or loss at an interface, see Fletcher (this volume).]

The Broad Field

Using reference directions as in Figure 2, consider a line from the inclusion's center running north. As already shown, the profile of mean stress along such a line is as in Figure 7A. In absence of diffusion, if the inclusion is rigid, profiles of the north-south or radial stress and the east-west or tangential stress are as in Figure 7B (or if the inclusion is stiff but not rigid, see Figure 7C; here the separation distances p and q are in proportion with the materials' viscosities). In all three diagrams, for the mean stress the diminution outward (to northward) is proportional to $1/r^2$ and, in the manner of Figure 2B, the upward curvature along this

profile is exactly matched by a downward curvature of lines in and out of the page, --- the two curvatures balance. We now note that for the tangential stress, the upward curvature is clearly greater than for the mean stress and except right at the interface, the downward curvature is less; by contrast, for the radial stress, the upward curvature has been largely lost. Therefore, speaking geometrically, the tangential-stress surface has a net upward curvature and the radial-stress surface has a net downward curvature. If gradients on these surfaces separately drive diffusion, the tangential-stress variation will drive a net tangential accumulation outside the north part of the interface, and the radial-stress variation will drive a net radial loss; see Figure 7D. Along a line out to eastward, all the opposite effects occur, so that radial-stress variation drives a flux from north to east, whereas tangential-stress variation drives a flux from east to north. So far it remains true that no material element either swells or shrinks in volume, but in the north, there is radial shortening and tangential elongation while in the east, there is radial elongation and tangential shortening. It is reassuring to note that these are strains of the same type as are occurring simultaneously by viscous creep; anisotropic strain by diffusion adds to the deformation, it makes the material yield more readily; one sees greater strain rates and smaller stress peaks when this kind of diffusion is occurring than if diffusion were to act isotropically or not at all.

Figure 7. Stress profiles along the north axis



Stress profiles along the north axis and consequent gains and losses of material.

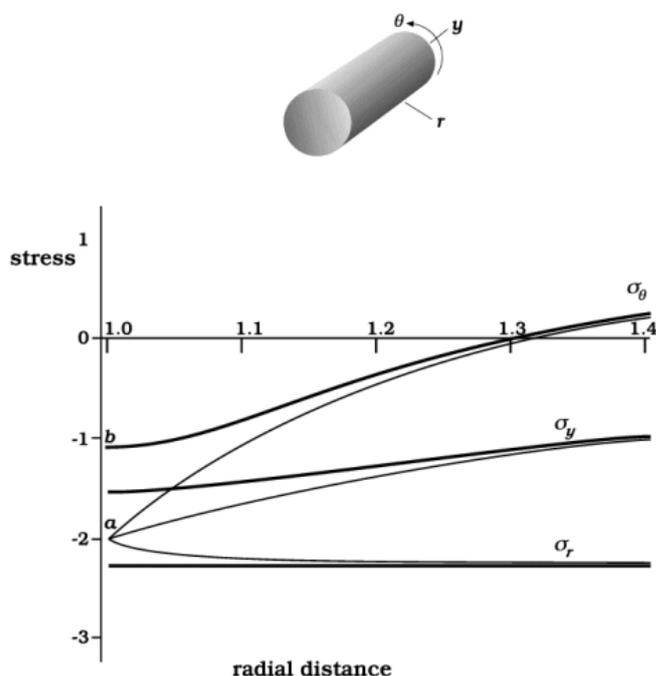
(One might ask, about the north region for example: if, as above, radial-stress variation drives radial loss of material and tangential-stress variation drives tangential gain, would not most of the material that moves simply "slip round the corner" without ever leaving the site? No, radial loss and tangential gain at the same location go on at whatever rate the viscosity permits, given the stress difference at that location. We are looking here at additional radial loss that occurs because the radial compression is lower on either side of the north point, at neighboring points just to the east and west.)

Details close to the inclusion

Two concepts were illustrated in Figure 5 for the region close to the cylindrical interface. Figure 5A suggests a discontinuity: the idea is that a film of newly-deposited material forms and separates the two regions whose stress fields etc. are described by the equations. In Figure 5B, by contrast, a change in the curvature of the stress surface is suggested. Such a stress field would lead to accumulation not at the interface but in the region close to the interface; material arriving from upstream would accumulate in a dispersed manner continuously throughout the material of the matrix in that region. The occurrence of augen suggests that Figure 5A is closer to what happens in deforming rocks, whereas Figure 5B is closer to what happens in many other instances of chemical diffusion. Actually, even in rocks, the loss of material by diffusion may occur in a dispersed, quasi-continuous manner; it may be only the gain or deposition process that is localized in well defined pockets. Anyway, setting reality aside, the theoretical work I wish to extend (Fletcher 1982; Stephenson 1988; Finley 1994) is more in the manner of Figure 5B and therefore a description more like 5B than 5A was sought.

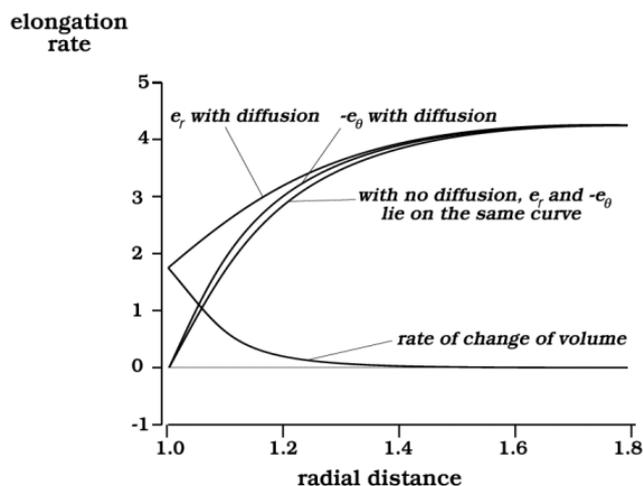
The relevant equations are given in Appendix 3, and some of the results are shown in Figures 8 and 9. Figure 8 shows stress magnitudes along a radial line to the east in the direction-system of Figure 1. The effects of diffusion are greatest close to the interface. Again the effect is to diminish and smooth out peaks and extreme values; in particular the tangential compression σ_θ no longer drops to such an extreme value. The change of curvature proposed in Figure 5 is seen: concave-upward curvature is noticeable in σ_θ and perceptible in σ_y . By themselves, these upward curvatures would lead to accumulation of diffusing material and elongation in the tangential and y-directions. However, the theory assumes a totally coherent interface: the matrix is taken as firmly glued to the rigid inclusion and cannot elongate at the interface except radially outward. Instead of causing lateral swelling, then, the influx of diffusing material leads to a stress build-up e.g. from a to b in Figure 8; the material still swells, but constrictive stresses force the effect to occur by radial elongation.

Figure 8. Stress profiles along the east axis



Light lines are profiles unaffected by diffusion; in that condition, σ_y and the mean stress are equal so the curves here match Figure 7 (inverted) and Figures 5 and 2. Heavy lines show modified stress profiles such as might be present when diffusive transport occurs and gives unequal contributions to the strain rates radially and tangentially. In particular, the concave-upward part of the profile for σ_θ leads to accumulation of material and a tendency toward tangential elongation, but this is exactly countered by σ_y now being greater than σ_r and σ_θ which by itself would give tangential shortening. Compared with the light-line profiles, the change in magnitude of σ_θ and the change in curvature have to have equal and opposite effects on the tangential strain rate, if the matrix is to remain coherent with the inclusion.

Figure 9. Strain-rate profiles along the east axis.



The matrix swells, gaining material by diffusion, but because of being coherent with the rigid inclusion, at the interface the swelling is entirely by radial elongation.

The strain-rate consequences are seen directly in Figure 9. The radial elongation ϵ_r is noticeably larger when diffusion operates, whereas the tangential shortening hardly changes. Of course the latter is artificially pinned at zero at the interface by our assuming perfect coherence. With this constraint, it appears that as far out as 1.5 or 1.6 on the radial scale, the tangential shortening is actually a little greater when diffusion operates, as if the stress field overcompensates; but the equations are only a coarse approximate solution, and this detail in the curves for eq may be insignificant. The more important point is that we now see unequal strain rates in the radial and tangential directions, and increases of volume due to diffusion that are distributed through the matrix in a continuous manner rather than as a discrete sliver of new material at the interface.

Numerical values

Figures 8 and 9 show differences between behavior when diffusion is occurring and when it is not. The differences are easily seen and are linked to important concepts, but in the particular example calculated, they do not amount to a large change in the overall strain field. This conclusion can be illustrated in geological terms as follows.

Let the rigid inclusion be a chert nodule in limestone, idealized to a circular cross-section of diameter 2 cm and a much greater length. Let the limestone be deformed, for example in the hinge of a fold, so that a region around the nodule is changed from a 10-cm square to a rectangle 6.25

cm by 16 cm. We focus attention on points 5 mm out from the nodule boundary, or 1.5 cm from its centerline. If the nodule were as readily deformable as its matrix, in the direction of maximum elongation such a point would move through 9 mm to end 2.4 cm out. If the nodule is rigid and no diffusion occurs, the motion would be reduced to 1 mm; a rigid nodule powerfully inhibits deformation of its immediate surroundings. Now let diffusion run, with stresses as in Figure 8 yielding strain rates as in Figure 9: the outward motion of the point in view would increase only about 14% --- an extra motion of only a fraction of a millimeter during the total episode of deformation. This small change is of course tied directly to the particular example described in Appendix 3, and specifically to the value of the characteristic length L in that example ($0.188 \times$ the inclusion radius). If L had a larger value, the effect of diffusion would be greater; even so, part of the effect is to reduce the stress concentrations; the effect of diffusion does not appear wholly in the form of enhanced strain rates.

Need we look at actual stress magnitudes and duration of the deformation episode? No, the length L is the essential parameter. Suppose (unrealistically) that the change in dimensions of the reference square from 10 cm to 16 cm occurred at a constant strain rate of $3.10 \cdot 10^{-14}$ per sec for (6.7) 1012 sec, in a rock of effective viscosity 1020 Pa-sec; then the driving stress difference must have been 12 MPa, and the diffusion coefficient $K = 9 \cdot 10^{-27} \text{ m}^2 \cdot \text{Pa}^{-1} \cdot \text{sec}^{-1}$, (from $L^2/4N$). Now suppose the temperature or the pore-fluid chemistry were different so that the effective viscosity was only half as much: the time for the deformation would change, but experience indicates that K would increase by a factor close to 2 --- (K and N varying inversely), --- so that L would not change and, like the total strain, the same total diffusive effect would be gained at twice the rate in half the time.

Discussion and conclusions

The main idea inspected is: when material is gained or lost by diffusive mass transfer, the gain or loss need not be the same in all directions; inside even an isotropic continuum, a small spherical element can be changed to an ellipsoid by unequal diffusive gains or losses as well as by the more commonly envisaged process of deformation at constant volume.

A more careful statement of the same idea is as follows. Suppose that at some point in the material, the deformation at some moment can be described using a strain-rate tensor:

then if the material is both viscous with viscosity N and self-diffusing under stress with coefficient K , the total strain-rate tensor can be partitioned into a first part controlled by N and the stress state at the point, and a second part controlled by K and the variation in stress around the point. The main idea in view is that the latter part of the strain-rate tensor need not be isotropic and in general will not be. By contrast, a different idea also considered in the body of the paper is that the K -related second part is necessarily isotropic, i. e. gain or loss of material by diffusive mass transfer can change a spherical element only to a larger or smaller sphere.

In parallel with the two ideas about the mass-transfer part of the strain-rate tensor, there are two ideas about the driving gradient. One can consider the gradient through space of just the mean stress (which has a single value at any point considered) or one can consider the gradients through space of several separate stress components. The version using mean stress goes with the idea that a sphere changes only to another sphere. I have tried to show that one can make a certain amount of progress using either version, mean stress plus isotropic strain by mass transfer OR full stress state plus anisotropic strain by mass transfer; Figure 4 and Appendix 1 are based on the first version, and Figures 8 and 9 and Appendix 3 on the second.

The two versions just discussed both treat diffusive mass transfer through the body of the material, but there is also the option of considering diffusive mass transfer only at bounding surfaces or interfaces (see Fletcher, this volume). When applied to a fold or a boudin, this approach is quite different from considering the interiors of rock units in the manner of the present paper; but if one considers the grain interfaces inside an extensive body of granular rock and then averages over many grains, the resulting equations have much in common with those for the interior of a continuum. Fletcher (1982) took this approach and, in course of averaging, took the mean-stress/isotropic-strain-rate option for gains and losses by diffusive mass transfer (1982, p. 278,279). I believe that no theory has yet taken the parallel path, combining attention to interfaces with the anisotropic-strain-rate option, despite the fact that rock thin-sections contain abundant features prompting thoughts in that direction e. g. intergranular seams of insoluble material that appear to be residues.

It might seem that a continuum theory is basically different from any theory built by treating a rock unit as a mass of grains separated by interfaces, but the difference is not

as great as at first appears. Macroscopic experiments designed to give estimates of N and K ignore whatever microstructure a real material may have, but as discussed in the main text and in Appendix 2, any pair of experimental values for N and K defines a characteristic length L for the material. I believe this length L , of the order of nanometers or micrometers, arises from the real material's microstructure; then if, in a theory, we postulate that a continuum has properties N and K , we implicitly suggest that the continuum has some kind of microstructure. The difference is that in the "continuum theory" we suggest nothing about what the microstructure is, and make no distinctions such as that between interfaces and grain interiors. But in Fletcher's approach, after individual grains have been considered, the averaging step smoothes over the geometrical details of the interfaces and solid grains. So in the granular treatment, the microstructure is specified but smoothed over, whereas in the continuum treatment, a microstructure is not specified but is implied. The two approaches are complementary and illuminate each other.

On the other hand, a difference between two basic ideas remains. Whenever there is diffusive mass transfer from a high-compression source toward a low-compression sink, we suppose that the flux is linked to some kind of stress gradient. One version holds that at any point in such a gradient, the relevant quantity is a single stress magnitude; the other version holds that in general all three principal stress magnitudes are relevant and that it is only when attention is confined to diffusion along a surface that a single stress magnitude per point suffices. To insist on a single value at each point or to admit a suite of values at each point are two fundamentally different ways of proceeding.

The same two options are current regarding chemical potential. The idea that a component's chemical potential can have only one value at a point is of rather long standing; the second idea, that in a stressed material the potential has a suite of values at a single point, was proposed by Ramberg (1959; for the same proposal in a more accessible journal, see Ramberg 1963). Independently Bowen (1967, 1976) proposed a chemical potential tensor, with principal values conforming to Ramberg's definitions. A strong endorsement of this approach is given by Grinfeld (1991, p. 2 and 132). Most interestingly, Green (1986) uses Bowen's tensor (Green's symbol G_{ij} , p. 202) but states that "it would be misleading to call G_{ij} the Free Enthalpy tensor because the Free Enthalpy is a scalar quantity." Having recognized the

tensor, he directs attention strictly to an interface and uses only a single component from it.

Conclusions We take pure shear of a highly viscous cylinder in a less viscous matrix as a sample problem where diffusive mass transfer may occur. Fletcher (this volume) approaches the problem assuming diffusion only along the interface, while Finley (1994,1996) approaches it assuming only volume-diffusion. There is no incompatibility here; in a real situation, diffusion is likely to run both at the interface and through the volume, and the separate treatments are useful steps toward something more comprehensive.

In the present paper, two more treatments are offered, both emphasizing volume diffusion, both incomplete. In the first, we assume that diffusive mass transfer is driven by a gradient in the field of mean-stress magnitudes; in the second, we assume that gradients in several separate stress components need to be considered for a full analysis of diffusion effects. The conclusion is that both approaches deserve attention and need more work. (A fifth approach (Bayly and Minkel, in press) uses finite elements and explores further details.) The problem turns out to be quite intricate but a benefit is that it encourages attention to a number of behaviors that will reappear in other geometrical configurations. My personal expectation is that for volume diffusion, using several separate stress components will gain acceptance as being fundamentally correct, but that in many instances, using just the mean stress will be a wholly satisfactory approximation. Also diffusion at interfaces governed by the interface normal stress will in many situations be more important.

Facts so far ignored are that any real inclusion differs from its matrix in both composition and density. Consequences of a density contrast are explored by Green (1986)

and consequences of variable composition by Bayly (1992, chapters 15 and 16). Consequences of the high mobility of cations compared with components of the Al-Si-O substrate are noted by Bayly (1987 p. 577, 578). A corollary is that hydrogen ions (protons) will tend to diffuse toward high-compression sites and mobilize oxygen atoms there by detaching them from the substrate. Overall, much remains to be done; there are many avenues to explore.

In concluding I revert to the fact that in this volume we honor Win Means' contributions. His demonstrations of what can be learned from bench-top analogs are a continuing source of insights and stimuli. A photographic record of some augen growing may soon be available to guide the construction of relevant theories and to strengthen the link to behaviors in real rocks.

Editor's Note

Note that this special volume is also preserved in its original format.

To see this paper in that format copy the link below into your browser

<http://virtualexplorer.com.au/webroot/special/mean-volume/contribs/bayly/index.html>

or click on the link provided here.

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During preparation of this paper, Hans Ramberg died, scholar and friend.

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A. Appendix 1: An embedded cylinder in pure shear

The remote stress field shown in Figure 1 has principal stresses $M+S$ and $M-S$, imagined as compressions. Eventually we shall want to consider the interface to be coherent and an overall compression M helps to make this plausible. But such an overall compression has no effect on the deformation or the associated stress variations; these can be fully discussed with remote principal stresses of S and S' , without the M . Additionally, for algebraic purposes it is convenient to have elongation rates as positive and hence to have tensile stresses as positive also; thus we consider a tension S to east and west and a compression S' from north and south. We use polar coordinates (r,q) with the interface at $r = 1$ and the direction of maximum tension as $q = 0$.

A solution of the corresponding elastic problem in absence of diffusion is given by Muskhelishvili (1963) and followed by Jaeger and Cook (1979), but their powerful general method is not readily extended to conditions that include diffusion. By contrast the following method is of narrow application but can be extended so as to shed light on diffusive behavior.

Assume that the stress field can be described by a series of terms of the form $A.r^N.\cos mq$; then for reasons of symmetry, m must be an even integer. Also, stress magnitudes must not become infinite at $r = 0$, so that inside the

inclusion, no term can have N negative; similarly, stress magnitudes must not become infinite at remote points (∞) so that outside the inclusion, no term can have N positive.

To narrow the range of possibilities farther, it is convenient to look at a different term $B.r^n \cos m\theta$ and to name it f . The convenience lies in the fact that if we put

[1a,b,c]

we automatically conserve momentum and describe steady flows, with no accelerations. Specifically for $f = B.r^n \cos m\theta$,

[2a,b,c]

If the material remains continuous, it will also be true that

[3]

where e_r and e_θ are linear strain rates and g is the engineering shear strain rate (twice the tensor shear strain rate). For a Newtonian material of viscosity N ,

[4a,b,c]

Let the direction of the cylindrical inclusion's long axis be y . Then if $e_y = 0$ (plane strain),

[4d,e]

If [2a,b,c] are used in [4c,d,e], the continuity equation [3] shows that

[5a,b]

In particular, for variation specifically with $\cos 2\theta$, $m = 2$ and $n = 4, 2, 0$ or $2'$.

Because of the restrictions on the powers of r in the stress terms, N or $n-2$ as discussed above, we conclude that inside the inclusion $n = 4$ or 2 and outside the inclusion $n = 2, 0$ or $2'$. For the value $n = 2$, the r -dependence drops out of the stress terms; the pair $m = 2, n = 2$ describes just a homogeneous stress field such as would exist throughout the entire region if the inclusion were mechanically no different from the matrix.

The conclusion so far is that for the interior of the inclusion, a possible form is

[6a]

and for the exterior,

[6 b]

where a, b, d, f and g are coefficients yet to be determined. At once, d is fixed by the stress state as r becomes infinite: at $q = 0$, $sr(\infty) = S$ so, from equation [2b], we need $d = -S/2$. The remaining coefficients a, b, f and g can be chosen according to whatever conditions we wish to satisfy at the interface.

The classical conditions at the interface are:

equal stresses, $(sr)_i = (sr)_e$ and $t_i = t_e$, [7a,b]

and equal velocities (to maintain coherence),

$u_i = u_e$ radial and $v_i = v_e$ tangential [7c,d].

These yield

[8a,b,c,d]

where R is the ratio $(\text{viscosity})_i / (\text{viscosity})_e$. Putting these expressions into (6a) and (6b) gives the same stress functions as are derived by Muskhelishvili (1963). In particular, the value $a = 0$ corresponds with the notable fact that the stress field throughout the inclusion is homogeneous, and this value of a is derived specifically from the interface conditions given. Any other interface conditions are likely to yield a non-zero value for a and an inhomogeneous stress field in the inclusion.

From the main text, we would like to find interface conditions that would allow for the material diffusing away from the north and south quadrants of the interface and accumulating at the east and west quadrants. To allow the radial velocities u_i and u_e to be unequal is an obvious choice; then at the east point, for example, a gap opens at the rate $u_e - u_i$ and we can seek a balance between this rate and the rate at which material is arriving by diffusion. But once the process of deposition at the interface gets under way, it is not at all clear how the other interface conditions (7a, b and d) would change. For present purposes, we focus attention on just the moment when deposition begins, when the deposited film or sliver is infinitesimally thin, and propose that at this moment conditions (7a, b and d) can still be applied.

This is clearly just a first step toward a more realistic analysis.

With u_i and u_e unequal, we can introduce b where $u_e = b \cdot u_i$ and now find:

as before, [9a,b,c,d].

If we use these values to estimate and close to the interface and assume that the diffusivities of inclusion and matrix are also in the ratio R ($K_e/K_i = R = N_i/N_e$), we derive for any interface point:

[10a,b,c,d]

Also,

[11]

so the diffusive fluxes take care of the excess or deficit at the interface if

[12]

The product $4K_i N_i = L^2$ where L is a characteristic length of the material of the inclusion. Thus for example for $R = 10$, $b = 5/4$ if $L = 1/6$, or $b = 2$ if $L = 1/3$. Diffusion not only enables the matrix to deform more freely, it reduces the height of the stress maxima; for example, in the condition ($R = 10$, $L = 1/3$ and $b = 2$), the radial compression at the north point is about 0.8 of its magnitude without diffusion.

For larger values of b or R , the exact form [10c] has to be used, and as R tends to infinity and u_i tends to zero,

[13]

For example, if $L^2 = 0.2$, $u_e = S \cos 2q/6N_e$ or specifically at the east point, $u_e = S/6N_e$. (For comparison, if we replaced a rigid inclusion by material homogeneous with the matrix, then at the east point of a circle of radius 1 we should find $u_e = S/2N_e$). Again, diffusion allows the matrix to deform as if the inclusion were much less viscous than it is. In fact algebraically, if we put $L^2 = 1$ into equation (13), $u_e = S/2N_e$ as for a homogeneous material. But Appendix 2 shows that treating a material with microstructure as a continuum becomes increasingly unrealistic as L^2 increases above 0.1 or 0.2; it is more the qualitative trend in these results that is of value.

B. Appendix 2: The characteristic length L

For a physical picture of the length L , consider two compressive stresses s_1 and s_2 , and a small element of material that is part of, and embedded within, a larger extent. If s_1 is imposed on the element north-south and s_2 is imposed east-west, a north-south shortening strain rate will be present, --- $(s_1-s_2)/4 \cdot (\text{viscosity})$ in plane strain or $(s_1-s_2)/3 \cdot (\text{viscosity})$ with cylindrical symmetry. Now consider a different situation where one site within the material is compressed hydrostatically by s_1 and a site not far away is compressed hydrostatically by s_2 ; in this set-up, there is radial shortening at the high-stress s_1 site because of self-diffusion of material away to the low-stress s_2 site. The rate of radial shortening depends on the separation-distance of the two sites, and there is some separation distance such that the radial shortening rate by self-diffusion equals the viscous shortening rate in the first situation. This particular separation-distance is the length L (or, in some formulations, a small multiple of it such as $L/2$).

In most practical situations, L is less than a micrometer. In fact, there is an inherent awkwardness: the manner in which L is defined above assumes that the material is ideally continuous, whereas both creep and self-diffusion depend on the material having microstructure, such as atoms and dislocation loops; and L is so short that, on the scale of L , one sees the microstructure, --- one cannot reasonably treat the material as a continuum.

A resolution is as follows: we admit that every material is atomic; this includes admitting that "homogeneous" plane strain involves atoms moving around, dislocation loops expanding or shrinking and so on; then in homogeneous plane strain, there is an average distance an atom moves in contributing to the strain process. Where the dominant mechanism is dislocation-climb, for example, the average distance would be of the order of magnitude of the length of a dislocation or the separation of one dislocation from the next. A second view is that L is an estimate of this average distance.

Fortunately, the two views of L are, I think, wholly compatible. If one works wholly at the macro-scale using material slabs as in Figure 6, one can measure viscosity N and diffusivity K , respectively in Pa-sec and $m^2\text{-Pa}^{-1}\text{-sec}^{-1}$.

Then $(4NK)^{1/2}$ is a distance, --- determined macroscopically but informing us about the microstructure; I think it tells us the average distance a participating atom moves when the material undergoes homogeneous deformation, or is a good indicator of that distance.

(Of course, $(NK)^{1/2}$ --- without the 4 --- is also a distance. As a purely technical point, to define L as $(4NK)^{1/2}$ leads to neater equations, but currently estimates of K are so uncertain that the factor of 4 has no practical significance.)

A third view of L or L_2 is gained if we use the idea of a material's mobility m , with $m = 1/N$. Then $L_2 = 4K/m$ or $m = 4K/L_2$. For an atomic material with self-diffusion coefficient K , the shorter the distance L that an atom has to travel in contributing to change of shape, the greater the mobility m with which the material will deform.

C. Appendix 3: Anisotropic gain or loss

The whole of Appendix 1 rests on the observation that in the classical description of stresses around a cylindrical inclusion, If one's assumptions about diffusion are:

conservation of volume, i.e.

linear strain rate e or $dV/V.dt = (dV/V.dt)/3$ in all directions,

(with elongations and tensile stresses positive) then whatever fluxes might be driven by gradients in the mean stress in the classical description, they would flow through the material without changing any dimensions, and would affect the stress field only by affecting conditions at the cylindrical interface. The purpose of this appendix is to explore the following alternative assumption: in place of

for all directions, we postulate

[1a,b,c]

(which leave the volume strain rate as before). These, of course, are only the parts of the strain rate due to diffusion; if the material also creeps with viscosity N , the total effects are:

[2a,2b]

etc.

The intention is to pursue the ambition illustrated in Figure 5 using these alternative rheological assumptions.

[The postulates (1a, b, c) have been derived from fundamental concepts elsewhere, in a skeletal manner (Bayly 1988, 1996) and at greater length (Bayly 1992), and the associated flow law or constitutive relation is shown in Supplement 3. Here the ambition is not to advocate but merely to test the postulates by results: can they yield a stress field, a strain-rate field and a pattern of diffusive fluxes? If they can, do the results "look reasonable"?)

As in Appendix 1, we use polar coordinates, seek a stress function j rather than seeking the stresses themselves directly, and imagine a series of terms in j for any of which $B.rn.cos\ m\ q$ can be taken as representative. As before, derived stresses are

[3a,b,c]

(conserving momentum), and again we wish to use the strain-rate relation that exists for any continuous velocity field,

[4]

To use this relation, we need expressions for e_r , e_q and g , for which we need in turn expressions for σ_r and σ_q and for the shear-strain consequences of the diffusion postulates in equation-set [1].

For a single-valued scalar variable f , in polar coordinates is

but sr is not a single-valued scalar: it is a scalar component of a tensor and thus a multivalued direction dependent scalar.

Then:

[5a,b,c]

(see Supplement 1 below). For a term $B.rn.cos\ m\ q$ in j these yield:

[6a,b,c]

To use these relations, one can seek a suitable series of terms in j , as in Appendix 1 at equations [6a and b]. For any such series, stresses in the (r,q) plane can be derived using equations [1a-c] of Appendix 1. But in a material with self-diffusion, equations [4d and e] of Appendix 1 cannot be reached; the plane-strain condition no longer establishes

$sy = (sr+sq)/2$; it yields only an equation like equation [2b] above, viz.:

[7]

for plane strain. Hence one needs to seek not only a suitable series of terms for j but also a suitable separate series for sy , such that in combination with each other the results satisfy the geometrical relation [4] and the boundary conditions. Both series are likely to be infinite, and to find such a pair by analytical methods is a difficult task, not attempted here. Instead, for purposes of illustrating the problem, just two extra terms are added to j and two to sy . With these additions, the plane-strain condition is almost satisfied, and for geometrical continuity only a slight degree of material anisotropy is needed. Further comments on the usefulness and weaknesses follow the presentation of the results themselves. Even for this elementary approach, the problem was further simplified by taking the inclusion to be wholly rigid and non-diffusing; it is only the behavior outside the inclusion that we try to describe.

An approximate solution

The solution explored is:

Basis for the solution The terms multiplying $\cos 2q$ are the classical solution for a non-diffusing material. One can assume that diffusion effects will be stronger closer to the cylindrical interface and weaker far from it, so that higher powers of r will be needed in the added terms. Along with higher powers of r , higher powers or multiples of $\cos 2q$ seem appropriate, and $\cos 6q$ is the first multiple that satisfies the symmetry requirements in Figure 1. Using even powers of r is simply an algebraic convenience; choosing which powers to use is a matter partly of subjective judgment (see also the Discussion section below). Once powers of r have been selected, the numerical factors are fixed by four conditions as follows: (1) if the inclusion is non-diffusing, there can be no diffusive flux across the interface; if sr , sq and sy are taken to be independent agents each driving its own flux, we need three separate conditions at the interface:

[10a,b,c]

(2) Although in the matrix generally, plane strain is achieved only approximately, at the interface we can satisfy that condition exactly.

Corollaries of the solution Profiles of sr , sq and sy are shown in Figures 8 and 9. The expressions derived from j are:

[11a-g]

These satisfy the boundary conditions $ey = eq = 0$ at $(r=1, q=0)$ if the material's characteristic length L is 0.188 times the inclusion's radius, or $L2 = 4NK = 0.0354$. With these expressions, the linear strain rates follow from equations like equation [2].

To assess the quality of the approximate solution in view, one can look at the two conditions we wish to satisfy. First, we seek plane strain: ey should be zero not only at the interface but at all values of r and q ; see Figure A3.1. Second, we have to maintain geometrical continuity in the material, in its velocity field; that is, the strain rates should satisfy equation [4]. On the left of this equation, g is linked to t through the material's shear viscosity, whereas on the right the linear strain rates eq and er involve the stretching or shortening viscosity. In principle, whatever the stress fields, one can satisfy [4] by postulating just the needed material properties at every point, but for realism, we wish to rely on this artifice as little as possible. That is, if we make the trial for an isotropic material, we wish to find the left-hand side of equation [4] not very different from the right-hand side. Figure A3.2 shows the comparison for $q = 0^\circ, 15^\circ$ and 30° ; at 45° , both sides of the equation go to zero and higher values of q merely repeat the same sequence of comparisons. The agreement is not as close as one would wish; I imagine a more accurate solution would involve more powers of r and other multiples of q ; but I also imagine that the extra algebraic complexity would not bring new principles to light; the present solution serves as regards bringing the needed principles into play.

Figure A3.1 Deviation of ey from plane strain.

Figure A3.2 The two sides of equation [4] compared, assuming that the material in view is isotropic.

[An obvious extension would be to admit diffusion and viscous creep in the inclusion as well as in the matrix, as in Finley's study (1994), but this too would not involve new principles.]

Discussion Two aspects are touched upon, namely, the choice of powers of r in the trial solution [8] and [9] and a desirable refinement of equation-set [1].

As regards choice of powers of r , a point not yet made is that the one-dimensional solution is available as a guide: if the radius of the inclusion tends toward infinite while the characteristic length L remains fixed, conditions just

outside the interface approach those at a planar interface, which are better known (Fletcher 1982; Bayly 1992 chapter 13). Specifically, at a planar interface, the rates of exponential diminution of stress away from the interface can be examined. As already remarked, when diffusion operates, we lose the simple relation $s_y = (s_x + s_z)/2$ or $(s_r + s_q)/2$ and s_y diminishes at its own rate with distance. In an appendix to chapter 13, it is shown that s_y diminishes less rapidly outward than s_z , and this fact led to smaller negative powers of r being used in equation [9] than in equation [8].

Secondly, in traditional uses of a Laplacian operator, the operand, for example temperature, is totally free of directional properties; but when the operand is directional, as in equation-set [1], the following seems desirable: in place of one should write,

[12]

The distinction of J from K was not made earlier for the sake of simplicity, but logically it is a distinction that must be made.

Basis for the solution

An Approximate Solution

The solution explored is:

Basis for the solution The terms multiplying $\cos 2q$ are the classical solution for a non-diffusing material. One can assume that diffusion effects will be stronger closer to the cylindrical interface and weaker far from it, so that higher powers of r will be needed in the added terms. Along with higher powers of r , higher powers or multiples of $\cos 2q$ seem appropriate, and $\cos 6q$ is the first multiple that satisfies the symmetry requirements in Figure 1. Using even powers of r is simply an algebraic convenience; choosing which powers to use is a matter partly of subjective judgment (see also the Discussion section below). Once powers of r have been selected, the numerical factors are fixed by four conditions as follows: (1) if the inclusion is non-diffusing, there can be no diffusive flux across the interface; if s_r , s_q and s_y are taken to be independent agents each driving its own flux, we need three separate conditions at the interface:

[10a,b,c]

(2) Although in the matrix generally, plane strain is achieved only approximately, at the interface we can satisfy that condition exactly.

Corollaries of the solution Profiles of s_r , s_q and s_y are shown in Figures 8 and 9. The expressions derived from j are:

[11a-g]

These satisfy the boundary conditions $e_y = e_q = 0$ at $(r=1, q=0)$ if the material's characteristic length L is 0.188 times the inclusion's radius, or $L^2 = 4NK = 0.0354$. With these expressions, the linear strain rates follow from equations like equation [2].

To assess the quality of the approximate solution in view, one can look at the two conditions we wish to satisfy. First, we seek plane strain: e_y should be zero not only at the interface but at all values of r and q ; see Figure A3.1. Second, we have to maintain geometrical continuity in the material, in its velocity field; that is, the strain rates should satisfy equation [4]. On the left of this equation, g is linked to t through the material's shear viscosity, whereas on the right the linear strain rates e_q and e_r involve the stretching or shortening viscosity. In principle, whatever the stress fields, one can satisfy [4] by postulating just the needed material properties at every point, but for realism, we wish to rely on this artifice as little as possible. That is, if we make the trial for an isotropic material, we wish to find the left-hand side of equation [4] not very different from the right-hand side. Figure A3.2 shows the comparison for $q = 0^\circ, 15^\circ$ and 30° ; at 45° , both sides of the equation go to zero and higher values of q merely repeat the same sequence of comparisons. The agreement is not as close as one would wish; I imagine a more accurate solution would involve more powers of r and other multiples of q ; but I also imagine that the extra algebraic complexity would not bring new principles to light; the present solution serves as regards bringing the needed principles into play.

Figure A3.1 Deviation of e_y from plane strain.

Figure A3.2 The two sides of equation [4] compared, assuming that the material in view is isotropic.

[An obvious extension would be to admit diffusion and viscous creep in the inclusion as well as in the matrix, as in Finley's study (1994), but this too would not involve new principles.]

Discussion Two aspects are touched upon, namely, the choice of powers of r in the trial solution [8] and [9] and a desirable refinement of equation-set [1].

As regards choice of powers of r , a point not yet made is that the one-dimensional solution is available as a guide: if the radius of the inclusion tends toward infinite while the characteristic length L remains fixed, conditions just outside the interface approach those at a planar interface, which are better known (Fletcher 1982; Bayly 1992 chapter 13). Specifically, at a planar interface, the rates of

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Secondly, in traditional uses of a Laplacian operator, the operand, for example temperature, is totally free of directional properties; but when the operand is directional, as in equation-set [1], the following seems desirable: in place of one should write,

[12]

The distinction of J from K was not made earlier for the sake of simplicity, but logically it is a distinction that must be made.

Corollaries of the solution

An Approximate Solution

The solution explored is:

Basis for the solution The terms multiplying $\cos 2q$ are the classical solution for a non-diffusing material. One can assume that diffusion effects will be stronger closer to the cylindrical interface and weaker far from it, so that higher powers of r will be needed in the added terms. Along with higher powers of r , higher powers or multiples of $\cos 2q$ seem appropriate, and $\cos 6q$ is the first multiple that satisfies the symmetry requirements in Figure 1. Using even powers of r is simply an algebraic convenience; choosing which powers to use is a matter partly of subjective judgment (see also the Discussion section below). Once powers of r have been selected, the numerical factors are fixed by four conditions as follows: (1) if the inclusion is non-diffusing, there can be no diffusive flux across the interface; if s_r , s_q and s_y are taken to be independent agents each driving its own flux, we need three separate conditions at the interface:

[10a,b,c]

(2) Although in the matrix generally, plane strain is achieved only approximately, at the interface we can satisfy that condition exactly.

Corollaries of the solution Profiles of s_r , s_q and s_y are shown in Figures 8 and 9. The expressions derived from j are:

[11a-g]

These satisfy the boundary conditions $e_y = e_q = 0$ at $(r=1, q=0)$ if the material's characteristic length L is 0.188 times the inclusion's radius, or $L^2 = 4NK = 0.0354$. With these expressions, the linear strain rates follow from equations like equation [2].

To assess the quality of the approximate solution in view, one can look at the two conditions we wish to satisfy. First, we seek plane strain: e_y should be zero not only at the interface but at all values of r and q ; see Figure A3.1. Second, we have to maintain geometrical continuity in the material, in its velocity field; that is, the strain rates should satisfy equation [4]. On the left of this equation, g is linked to t through the material's shear viscosity, whereas on the right the linear strain rates e_q and e_r involve the stretching or shortening viscosity. In principle, whatever the stress fields, one can satisfy [4] by postulating just the needed material properties at every point, but for realism, we wish to rely on this artifice as little as possible. That is, if we make the trial for an isotropic material, we wish to find the left-hand side of equation [4] not very different from the right-hand side. Figure A3.2 shows the comparison for $q = 0^\circ, 15^\circ$ and 30° ; at 45° , both sides of the equation go to zero and higher values of q merely repeat the same sequence of comparisons. The agreement is not as close as one would wish; I imagine a more accurate solution would involve more powers of r and other multiples of q ; but I also imagine that the extra algebraic complexity would not bring new principles to light; the present solution serves as regards bringing the needed principles into play.

Figure A3.1 Deviation of e_y from plane strain.

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D. Supplement 1 The Laplacian operator in polar coordinates modified

The Laplacian of a scalar field i.e. the divergence of the gradient, exists independently of any coordinate system. But frequently the field of scalar magnitudes is specified by means of a coordinate system, and the Laplacian at any point is evaluated by an algebraic expression using first and second derivatives with respect to the variables of position (x,y), (r,q) etc. At equation-set [5], Laplace functions are shown for the stress components s_r , s_q and t . The functions shown contain the standard terms for a two-dimensional scalar field in polar coordinates plus an extra term in each expression. The purpose of this supplement is to show how the extra terms arise.

First we rehearse in a diagram the source of the three standard terms; see Figure A3.3.

Figure A3.3 The neighborhood of a point P at which a Laplace function is to be evaluated.

To form the Laplacian of some single-valued function $f(r,q)$ at point P , we need the gradients of f along two orthogonal directions through P . The directions used are the radius and tangent through P . The radial gradient is f/r and its variation with r is $2f/r^2$. Let the tangential coordinate direction be s ; along s , we compare the gradients at

points X and Y in diagram B.

The new term arises at point P . Consider first the magnitude of s_r at point P : we wish to compare this with the normal-stress components on planes h , j and k in diagram A3.3C. For a single-valued scalar, distinguishing plane j

from plane h makes no difference, but with a stress component such as s_r there is a difference, namely; here the variable a is used for change of orientation at a point, as opposed to q where dq involves change of position as well as orientation.

From conservation of momentum we have so that for s_r , the gradient at X becomes

Also numerically, though not geometrically, $da = dq$; hence the extra term reduces to $2t/r$ and generates the extra term

$(-2/r^2).(t/q)$ in the Laplacian function.

The extra term for s_y is precisely similar. The extra term for t arises in a similar manner but uses the fact that

$$t/a = s_r - s_q.$$

For a useful check, we recall that the pair of values ($m=2$, $n=2$) in equations [6a,b,c] specify a homogeneous stress field, for which the three left-hand sides of equation-set [5] are zero by definition; when $m = n = 2$, the three right-hand sides do indeed vanish as needed.

E. Supplement 2: diffusion and shear stress

At equation [2b], the linear strain rate associated with s_x is composed of two parts, the viscous and diffusive contributions. But the expression of geometrical continuity [4] involves not only linear strain rates but also the shear strain rate g . In a non-diffusing material $g = t / N$ but again, admitting diffusion creates an extra term; the extra term, ϵ , is established as follows.

Let a small rectangular element carry stresses s_x , s_y and t as in Figure A3.4A; then the stress state can be described as a superposition of the two stress states shown in diagram B; here in magnitude the normal stress S equals the original shear stress t . Following the pattern of equation-set [1], we assume that the pair $(S, -S)$ drives linear strain rates and ϵ . These generate a shear strain rate in the element in diagram A with magnitude ϵ and because S and t are numerically equal, the shear strain rate is also

A fuller discussion of this topic is given in Bayly and Minkel (in press), as Appendix 2 of that work.

Figure A3.4 A general state of stress and an equivalent pair of pure-shear states.

F. Supplement 3: tensor expressions

To express the preceding ideas in a more comprehensive form, one needs to write the underlying constitutive relation thus:

in which C could have 729 components (a sixth-rank tensor). But in an isotropic material, C has a non-zero component only when $i=j$ and $k=l$, so the relation can be rewritten

(no summation)

with 27 non-zero components in C . With conservation of volume,

(summing over i) and if the material properties C are the same at every point,

The two coefficients that were noted in the Discussion section can be used again; thus when $j = k = i$, $C = J$ but when $j = k \neq i$, $C = K$ as in equation [12]. The ideas in Supplement 2 suggest further that when $j \neq k \neq i$, $C = K$ again but that when either j or $k = i$ (not both), C takes a third value designated H .

The viscous part of the strain rate is simpler:

where N is of fourth rank. Again in simple materials, N has a non-zero component only when $l = j$ and $m = k$. If one wished in a corresponding way to write:

M would have 81 components, but only 9 non-zero, any one term being of the form

and the triplets being JKK

HHK

HKH

HHK

KJK

KHH

HKH

KHH

KKJ .

In this approach, M bears some resemblance to N but in fact remains fundamentally different because M is not formed purely from material properties, it contains the second-derivative operators.