Considerations on the use of analogues in deformation studies

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Since Daubrée, experimental geology has used the concept of analogue materials in various senses, which will be critically reviewed here.

1 – Mechanical behavior (flow, folding, faulting) of microscopically homogeneous formations can be modelled by using analogue materials (plasticine, corn syrup. . .) with appropriate scaling (non-dimensional numbers). This approach has been illustrated by Ramberg.

 2^{-} Microscopic phenomena thought to be general and representative of important physical processes can be studied on materials more amenable to experimentation, such as metals or organic crystals. Thus, studies of the evolution of substructure (subgrain size, recrystallization) can shed light on the relevant processes and help calibrate palaeopiezometers.

3 - Elastic properties (sound wave velocities) of rocks and minerals can be scaled according to density and mean molar weight, allowing the extrapolation of properties of one mineral to higher pressures or the determination of the properties of one mineral from its place in velocity-density systematics (Birch).

4 - Microscopic studies on crystals of the same crystallographic structures can help build systematics and predict the unknown properties of a mineral, in general terms. The dislocations (although not their causes) are the same for all crystals of the same structure and there are fruitful similarities in creep or stress-strain curves. With proper scaling, isomechanical series can be found.

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Introduction

Deformation on the Earth takes place on such scales of space and time as to discourage attempts to study it by means of the methods of experimental physics; this is no doubt the reason why it was, and still is, largely approached by observation and speculation. The recognition that structural features like folds or faults, similar at all scales, must have been produced by similar processes, led early geologists like Sir James Hall to try and reproduce them in the laboratory. However, it was only at the end of the last century that Auguste Daubrée established "Experimental Geology" (Daubrée 1879) as a means of understanding tectonic processes through laboratory simulation and experimentation, using carefully selected analogue materials. Experimentation on "non-rock" analogues coupled with dimensional analysis has since been used to model large scale convective flow in the Earth's mantle as well as crustal tectonics - the latter aspect illustrated by Hans Ramberg's beautiful studies (Ramberg 1981).

The mantle and crust of the Earth are constituted of rocks, in turn constituted of minerals, which indeed, are the elementary bearers of deformation. Elastic deformation of mantle and core minerals, at pressures unattainable in the laboratory, propagates with seismic velocities inside the Earth, conveying information on its mineralogical constitution. However, to extract the information, it is necessary to know the elastic constants of the high pressure phases. Francis Birch (1961) showed that a fruitful approach was to derive the unknown values from systematics of the density-dependent seismic velocities determined on other minerals of *analogue* chemical composition.

Structural geology has recently extended its field of investigation down to the scale of the mineral crystals and geologists now use the optical and electron microscope to find microstructural imprints left by tectonic processes, that could be used as clues to guess at the temperature, pressure or shear stress prevailing when the rocks were deformed. As the physical processes of deformation are largely common to all crystalline matter, it has been found very useful to observe the formation of the microstructures, under known laboratory conditions, in *analogues* (metal, alkali halides, organic crystals) where they evolve more rapidly than in silicates or carbonates, while hopefully preserving the same relation to the physical parameters.

Finally, dynamical modelling of tectonic or geophysical processes such as mantle convection, requires that rheological equations for the materials be known. In some cases, they are known at ambient pressures and high shear stresses and must be extrapolated to much higher pressures and lower stresses; in other cases, when the crystals are stable only at mantle pressures and are unavailable for high temperature deformation experiments, one must resort to educated guesses as to the main characteristics of their rheological behavior. In both cases, deformation experiments on crystals with analogue crystal structure, coupled with electron microscopic examination of their lattice defects, provides a means, possibly the only one, to obtain some information.

In what follows, we will summarily review the various aspects of the use of analogue materials in terrestrial deformation studies, particularly concentrating our attention on those concerning microscopic plastic deformation processes.

Analogues and tectonics

Although he was not the first to try and reproduce the shapes of naturally deformed rock formations in the laboratory Daubrée was, to our knowledge, the first to introduce "Experimental Geology" as a respectable field in Earth Sciences (Daubrée 1879) and to apply the experimental method to the study of terrestrial deformation and fracture. He insisted that, in order to establish a correlation with observations of naturally deformed rocks, it is important to select appropriate substances to be stressed and he made it clear that the conditions are quite different for mechanical similarity and for geometrical similarity. Thus, although he did not formalize the selection rules for materials in terms of similarity, he clearly was a pioneer in the field of analogue studies, using various proportions of beeswax, plaster of Paris, resin and turpentine to obtain mixtures with mechanical properties ranging from extreme ductility to extreme brittleness, from which samples were fashioned and stressed in a hydraulic press (with the help of the engineer Tresca).

Most physical parameters (density, shear modulus, melting point) of the analogue materials can be controlled, as well as the external parameters temperature and shear stress, but it was recognized long ago that one cannot alter gravity (although this is now done in centrifuge experiments) and that this leads to inescapable constraints in dimensional analysis. Thus, Maillet & Blondel (1934) found that with the constraint of constant gravity and given that the density of most materials varies only between 1 and 5, the modelling of the rise of a mountain in 10 years instead of 10^7 years would lead to using a model of the Earth 0.04 mm in circumference! Hubbert (1937) and Ramberg (1981) established the bases of a rigorous dimensional analysis for hydrodynamic similarity (see also Weijermars & Schmeling, 1986).

The dimensionless parameters used in scaling analysis contain material constants of the analogue substance, so it is important to fully characterize it with respect to plastic properties, in various domains of temperature, strain rate etc. . . This has been done for modern analogue materials like plasticine (McClay 1976) and viscoelastic polydimethylsiloxane bouncing putties (Weijermars 1986). In the latter case it has been found that the nature and the amount of filler are responsible for the stress sensitivity of the strain rate (or stress exponent in power law creep) and the capacity for strain-softening. It is possibly the preferred orientation of the filler induced by rolling that causes the anisotropy in plastic behavior of plasticine noticed by Peltzer et al (1984): samples made of parallel layers of rolled plasticine deform homogeneously in uniaxial compression normal to the layers and exhibit localized shear zones and strain softening when compressed parallel to the layers: only in the last case is rolled plasticine an appropriate model for continental deformation by faulting.

These studies lead to the conclusion that correct dynamic scaling, indispensable as it is, is not sufficient to ensure an appropriate modelling of natural large scale deformation, the analogue material must also be fully characterized by using all the tools of materials science, and its microstructure investigated, as if it were a real Earth material. Last but not least, the analogue material must qualitatively behave in an appropriate way: eg deformation by faulting cannot be modelled with a newtonian viscous material. New analogue materials may have to be designed for specific problems. Thus, analogue modelling, already endowed with heuristic value, may truly become an irreplaceable tool in tectonic studies.

Analogues and microstructures

Microstructures of minerals in tectonically deformed rocks are currently observed with the techniques and methods of materials science, in order to obtain information on the deformation processes and the tectonic and/or metamorphic history of the rock: P-T path, maximum or latest shear stress etc. . . . Here too, analogues have an important part to play, but the analogy is of a different nature; it is based on the reasonable assumption that many important physical processes linked to deformation are not specific, that they exhibit general characteristics wherever they operate and that the microstructures produced can be read with a universal code. Thus, good analogues are crystals or polycrystals which allow easier observation of the relevant microstructure or for which evolution of the structure is more rapid and can be easily followed; their crystal structure and chemistry may be very different from that of the material they substitute for, but they must share the characteristics that governs the appearance of the microstructure under study.

For instance, quartzite is very difficult to deform experimentally and processes that become dominant at large strains, like preferred orientation or dynamic recrystallization, although important in nature, are almost impossible to study in the laboratory in certain temperature and stress regimes. Fortunately, there are interesting analogies between quartz and ice or hexagonal metals.

Ice is hexagonal, its principal slip systems are the same as those of quartz and as its optical characteristics are also similar, preferred orientation of grains of deformed ice can be studied in polarized light microscopy (as in quartz); the melting point of ice, however, is much lower so that high temperature deformation and large strains can be easily achieved. Ice has therefore been successfully used as an analogue of quartz (Wilson 1981).

Magnesium is an easily deformable hexagonal close-packed metal and although it is not transparent, the orientation of grains can be determined by optical microscopy in reflected polarized light; these qualities make magnesium a suitable analogue material for the microstructural study of large strain and the recrystallization of quartz rich rocks (Burrows et al 1979, White et al 1985, Drury et al 1985). Dynamic recrystallization is one of the most obvious structural evolutions accompanying high-temperature deformation. The interpretation of recrystallized structures and the use of recrystallized grain size as a "palaeopiezometer" to estimate the shear stress during deformation (see Poirier 1985) largely depends on the knowledge of the factors controlling the evolution of the structure (misorientation of subgrains, nucleation of new grains, grain boundary migration etc. . . .). Much of the knowledge we now have of the recrystallization processes in minerals has been obtained by experiments on easily

deformed and recrystallized ionic crystals like NaCl (Guillopé & Poirier 1979) or NaN03, an analogue of calcite (Tungatt & Humphreys 1981). Rapid unfolding of cycles of deformation, nucleation of small new grains or grain boundary bulging, grain growth etc. . . . has been witnessed in real time for low melting point organic analogue materials such as paradichlorobenzene (moth balls) (Means 1980), camphor (Urai et al 1980) or octachloropropane (Means 1983). The importance for deciphering the information hidden in recrystallized textures by watching the process taking place cannot be overestimated. This is also true of the localization of deformation in shear bands (Means 1980, Urai & Humphreys 1981). Experiments on low melting point, transparent, optically anisotropic organic materials of the kind used in the pioneering work of Win Means will no doubt be more systematically used.

Statistical treatment of the grain-size populations and correlation with creep curves at various stresses and temperatures, should also be done in a much more rigorous way. Indeed, paleopiezometry will not come of age unless serious data processing is done, taking into account such unavoidable facts as heterogeneity of dislocation population, multimodal distribution of recrystallized grain sizes or the various scales of subgrains.

Analogues and elasticity

Accumulation of elastic data from series of isochemical and isostructural mineral analogues defines trends. The elastic properties of an inaccessible Earth region (mantle or core) can then be ascribed to one or several minerals of the series.

Birch (1961) proposed a simple linear relationship between the velocity of P waves in silicates and oxides and the density ρ and mean atomic weight M:

$$V_p = a(M) + b\varrho$$

Velocity-density systematics can be established for minerals of different structures and chemical composition but having the same mean atomic weight; in other terms, the velocity of sound waves can be specified as long as M and Q are known. From this relationship, Birch drew the far-reaching conclusion that pressure affects the sound velocity of a mineral through its density, thus allowing the prediction of elastic constants for pressures too high to be attained in the laboratory. Birch's law is in effect an equation of state; Anderson (1967) proposed and theoretically justified a similar seismic equation of state that related the seismic parameter ϕ to the density: $\varrho = A(M) \phi^n$

 $(\phi = K/\varrho)$, where K is the bulk modulus, is equal to the square of the bulk sound speed).

Numerous other systematics were proposed by various authors. Shankland (1977) reviewed and analyzed them in terms of the physics of ionic and electronic interactions in the solids. Velocity-density systematics and Birch's law have been very helpful for interpreting seismic data in terms of mineralogical models of the mantle and they are the basis of one of the best arguments of the existence of an iron core.

Velocity-mean atomic weight systematics for compounds with the same crystal structures of unavailable mantle minerals but different chemical compositions can be used to predict the sound velocity (hence elastic properties) of these minerals. Thus, systematics on germanates and titanates isostructural with the high pressure silicates ilmenites or perovskites have been used to predict elastic properties of MgSi0₃ ilmenite or perovskite (Liebermann et al. 1977, Liebermann 1982).

Despite the very successful use of systematics of analogues, one must be aware of a possibility of indiscriminate use of elastic analogies. Indeed, comparison of compressional velocities of returned lunar rocks and various Earth materials seems to confirm the idea that the moon is made of green cheese (Schreiber & Anderson 1970).

Analogues and the Physics of Plasticity

In most cases plastic deformation is caused by glide of dislocations on dense crystallographic slip planes. The Burger vector of dislocations are vectors of the Bravais lattice. All crystals with the same Bravais lattice are in a way analogues in the sense that they have potentially the same dislocations and the same slip planes. The analogy however must be restricted to crystals of the same structure (in the sense of crystal chemistry), taking into account the type of bonding. Thus, although aluminium, sodium chloride and silicon are all face centered cubic crystals, they do not have the same dislocations or slip systems: for instance, aluminium slips easily as expected, on the densest planes of the (111) type, whereas sodium chloride slips on (110) planes which do not involve (as (111) planes would) any hindrance due to the electric charges of the ions. Important differences also appear in the splitting schemes of dislocations, energies of stacking faults, and core structures of dislocations, hence their mobility: dislocations in silicon are straight due to a high lattice

friction, whereas they are not very much crystallographically constrained and rather mobile in sodium chloride or aluminium.

It is then possible to identify isomechanical groups of materials having the same structure and similar bonding (Frost & Ashby 1982). Deformation-mechanism maps, constructed from experimental data, have an almost identical disposition of deformation mechanism fields (dislocation creep, diffusion creep etc. . . .) for materials of the same group when they are plotted in normalized coordinates (e.g. σ/μ , T/T_m), whereas they are clearly different from materials belonging to different groups. Thus for instance, crystals with the rock salt structure can be subdivided in 4 isomechanical groups: alkali halides, simple oxides, lead sulphide, metal carbides. There obviously are differences between materials of the same group, due to the possible existence of various distortions, as in perovskites, $BaTiO_3$ or $GdFeO_3$ – type distortions, or in hexagonal metals where dominant slip systems depend on the stacking fault energy on various planes, and in the last analysis, of the electronic structure (Legrand 1984).

Thus, there are several degrees of analogy which all have their own usefulness. The first degree, that of the crystal system, is not devoid of interest in that it allows the mapping of potential geometrical similarities (slip systems, Burgers vector) but it has no dynamical value. The second degree, that of the crystal structure, is more powerful and allows the study of many properties on more convenient analogues: crystal structure is indeed related to many physical properties, depending as it does on the interatomic potential.

Thus, good analogues of SiO_2 are BeF_2 , which has the same phase diagram as SiO_2 when plotted in T/T_m , or GeO_2 , which is a model of SiO_2 for high pressures. The melting curves of these structural analogues have been studied under pressure in order to better understand the behaviour of SiO_2 (Jackson 1976). Berlinite AlPO₄ is also a good analogue of quartz, in which dislocations and the role of water can be conveniently studied (Doukhan et al. 1987).

In the narrower third class of analogue materials one would find compounds with the same structure and a similar chemical composition. The purpose of studying these analogues is then essentially to establish systematics in their plastic properties. Thus, for instance it is interesting to study oxide perovskites such as BaTi0₃, KTa0₃, CaTi0₃ etc. . . . which are available at ambient pressure, in order, it is hoped, to predict quantities such as activation energies of creep for instance, for the mantle perovskite MgSi0₃. The approach here is similar to that followed for elasticity but the scaling parameters may be different (shear modulus or melting temperature for instance). Of course it might be necessary, as mentioned above, to distinguish subgroups according to the distortions.

One of course must bear in mind that analogy has its limitations and that a good analogue in one respect might be bad in another. For high-temperature plastic properties, the importance of the atmosphere (reducing or oxidizng) must not be neglected. Depending on the partial pressure of oxygen, an oxide or silicate containing a transition metal susceptible to take several degrees of oxidation like Fe or Co, do not necessarily behave as similar compounds containing only magnesium. The choice of the best analogues and the construction of reliable rheological systematics will no doubt be put on a more secure basis in the near future when ab initio calculations and computer simulation of dislocation cores using semi-empirical potentials become more widespread.

Also, in order to properly compare and calibrate the creep laws for the isostructural compounds used in systematics, one must be reasonably sure that the fit of the laws to the experimental data has been done in the same way, with comparable uncertainties and that the creep law fitted was the best in each case. This cannot be achieved by the traditional eye-ball fitting of straight lines on ln $\dot{\epsilon}$ - ln σ or Arrhenius plots. Use of modern data processing methods like global inversion should be encouraged (Sotin & Poirier 1984).

Conclusion

Analogy is probably a natural tendency of the human mind and although it can sometimes be misleading, its heuristic value has long be recognized. In Earth Sciences, analogue materials have been of great value and probably still will be for a long time, provided care is taken to perfect the way they are used. I suggest that this can be done in two opposite directions: For analogue materials used in large scale tectonic studies, whose use is already subjected to stringent quantitative scaling rules, progress might be achieved by paying more attention to their qualitative behaviour. On the other hand, qualitative microstructural investigations and palaeopiezometry or empirical systematics on analogues would benefit by a more quantitative treatment of the information, serious data processing and computer simulation.

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