accurate than two residue patterns, as expected. Third, current database size (75 proteins used here) appears adequate for two-residue patterns for which predictive results have plateaued, whereas it is woefully inadequate for three-residue patterns. Most three-residue patterns occur less than three times in the database and so cannot be used predictively at all. It is suggested that patterns should occur about 15 times for accurate prediction.

The authors make some reasoned speculations that approximately 1,500 protein structures are needed for accurate prediction. Even with a generous estimate of 50 structures being elucidated per year, this process will take more than 20 years. It is therefore reasonable to ask if there is any chance of improving predictions within the next 10 years, by which time we will probably know the sequences of more than 100,000 proteins. The general approach to structure prediction is shown in the figure.

Several areas look promising. Techniques for aligning sequences are being extended to recognize very distantly related proteins and allow model building on the basis of a known structure. The use of consensus templates is likely to be particularly powerful (see ref. 11 for a review). At one extreme, this method may be able to identify similar folds in unrelated proteins. The accuracy of structure prediction can be improved by using a family of homologous sequences[12], and this technique should be used where possible.

Qian and Sejnowski in the current issue[13] of the *Journal of Molecular Biology* show that neural network models, used previously for analysing speech patterns, can be applied to predicting secondary structure. The network model learns the relationship between sequence and structure from existing protein structures, and was then shown to give a 64 per cent accurate secondary structure prediction when applied to a test set of proteins. Qian and Sejnowski conclude that "no method based solely upon local information in the protein sequence is likely to produce significantly better results for non-homologous proteins".

In view of Rooman and Wodak's data, this conclusion seems unduly pessimistic. However, certainly the most obvious limitation of most prediction algorithms currently available is that they do not yet adequately address the problem of tertiary structure prediction or try to incorporate any of the knowledge currently available about supersecondary and tertiary folds (see, for example, refs 5,14). If we are to succeed before we have accumulated 1,500 protein structures, it will be necessary to encapsulate all our current knowledge including any available experimental clues. Structure prediction has remained elusive, but a problem of this importance deserves perseverence and perhaps we would do well to heed the following advice (with apologies to Piet Hein[15]):

The road to success? why its plain and simple to express
Err and err
and err again
But less
and less
and less. □

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Seismology

The fossil roots of continents

Peter Shearer

THE oldest rocks exposed at the Earth's surface are found on the continental shields, the stable central regions of continents, where they have remained relatively undisturbed for billions of years. But the longevity and extent of deeper continental structures is currently controversial[1,2]. Silver and Chan present seismic evidence on page 34 of this issue[3] that a 200-km-thick layer beneath the Canadian Shield has been stable for over 2.5 billion years. If their hypothesis is correct, this layer survived the breakup of the supercontinent Pangaea 180 million years ago and subsequent rafting of the layer over the underlying mantle by continental drift. This supports ideas that continents have chemically distinct roots to at least 200 km deep, which are mechanically strong because of their low temperatures and possibly because they are strain-hardened by ancient deformation.

Silver and Chan[3] examine the seismic phase 'SKS' recorded at nine stations in North America and Europe. This phase travels as a shear wave in the mantle, but as a compressional wave in the liquid outer core. Because of this path in the core, the polarization of the SKS wave at the receiver should always be parallel to the source–receiver azimuth. But Silver and Chan find that the arriving wave is often composed of two shear waves with different polarizations that arrive at slightly different times. This phenomenon, shear-wave splitting, is indicative of an anisotropic region within the Earth in which shear waves with different polarizations travel at different speeds. Shear-wave splitting has been observed in several studies[4–7] but rarely with the clarity of Silver and Chan's observations.

By examining earthquakes at various places around the globe, Silver and Chan show that the anisotropy must be located near each recording site. The time difference between the two shear-wave arrivals at station RSON on the Canadian Shield (Figs 1 and 2) is nearly 2 s and almost certainly arises from anisotropy in the upper mantle beneath the station. By analogy with measurements of crystal orientation in samples of upper-mantle material in ophiolites[8,9], Silver and Chan show that the most probable explanation for the anisotropy at station RSON is that the top 200 km of the mantle beneath the station contains olivine crystals which are aligned at an azimuth of N 75° E.

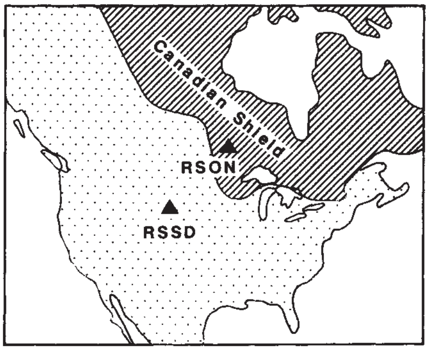

Fig. 1 Locations of the seismograph stations RSON on the Canadian Shield and RSSD in South Dakota.

Olivine crystals tend to become aligned in the flow direction during rock deformation[10]. The present motion direction of the North American plate at station RSON is not far from the observed anisotropy orientation. If the crystal alignment were related to the motion of the North American plate, the pattern of anisotropy should be relatively coherent over much of the plate, whereas Silver and Chan observe substantial variations in both magnitude and orientation of the anisotropy for stations only 1,000 km apart. They argue that a more probable explanation for the crystal alignment is the direction of the last significant deformation episode at each site. For station RSON, this occurred during the late Archaean (2.5 billion years ago) and the observed orientation of the Archaean geological fabric in surface rocks on the Canadian

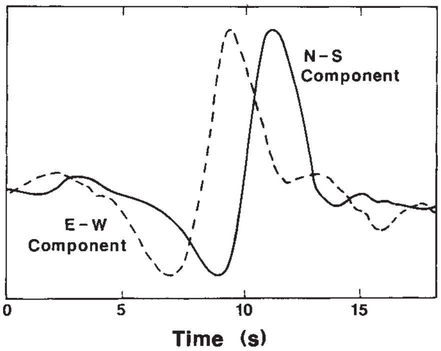

Fig. 2 Recordings from station RSON on the Canadian Shield show a 2-s delay between the arrival of the north–south and east–west components of the seismic phase 'SKS', caused by an anisotropic layer in the upper mantle beneath the station that splits the rising wave into two waves with different polarizations. In contrast, the splitting at station RSSD in South Dakota is only 0.6 s. (From Silver and Chan[3].)

Shield agrees with the anisotropy results. The observed orientation of the anisotropy at other stations also generally agrees with the grain direction for the last deformation event at each site.

The anisotropy observations at station RSON seem to show a crystal orientation which formed 2.5×10^9 years ago and has remained undeformed ever since. For this crystal fabric to have survived for so long, the mantle beneath RSON must be relatively cold, a result also suggested by observations of a high-velocity seismic root extending to a depth of 400 km beneath the Canadian[11] and Eurasian[2] shields. There seems to be a correlation between the thickness of the anisotropic layer and the presence of this high-velocity zone. At station RSSD in South Dakota (Fig. 1), where upper-mantle velocities are significantly less than at RSON[11], Silver and Chan calculate the anisotropic layer is only ~70 km thick.

These observations contradict models[12] in which the oceanic and continental temperature gradients are identical below 200 km. Instead, they support the theory that the low seismic velocities at depths of 200–400 km beneath the continental shields are related to temperature and compositional differences, and that this region moves coherently with the overlying plate[2,13]. But other geophysicists[1] maintain that temperature variations alone are responsible for the low velocities and that continental-plate motion is restricted to depths less than 200 km. (Details of these arguments were discussed by Thorne Lay in a recent News and Views article[14].)

Regardless of the eventual outcome of this dispute, Silver and Chan's results provide strong evidence that up to 200 km of the Canadian Shield have remained relatively undisturbed for billions of years. This stability suggests that the region is mechanically very strong and Silver and Chan speculate that this strength may be a result of the Archaean deformation itself. In a process analogous to the cold-rolling of steel, the rocks beneath the Canadian Shield may have been strengthened by strain-hardening.

These shear-wave observations of fossil seismic anisotropy are based on seismograms recorded at just nine stations. The results are so promising that the technique will certainly become widely used and eventually seismologists may be able to produce detailed maps of the ancient deformation of continents. □

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Conducting polymers

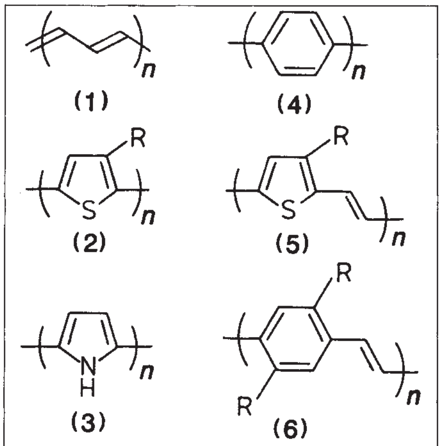
Seeing through synthetic metals

Martin R. Bryce

CHEAP, lightweight, durable and easy to make: these are the principal characteristics expected of polymer conductors that endear them to the electronics industry. Practice has not yet matched theory, but developments discussed at a recent meeting* suggest that there are grounds for hoping that polymers will replace metals as conductors in the next century. In particular, new, nearly transparent polymers have been synthesized that require less energy to excite electrons into the conducting state. Although these have lower conductivities than other polymers at present, they offer greater promise and are easily processed.

All organic polymers are intrinsic insulators, but high electrical conductivity in the range 1–500 siemens (S) cm^{-1} can be obtained when a conjugated organic polymer, that is one having alternating single and double bonds, is partially oxidized (p-doped) or reduced (n-doped) with suitable reagents — halogens and Lewis acids for oxidation; alkali metals for reduction. The usual polymers for these studies, polyacetylene (see 1 in the figure), polythiophene (2), polypyrrole (3) and poly-*para*-phenylene (4), are formed by electrochemical or chemical polymerization of the monomer units. By mechanically aligning the polymer chains of polyacetylene, conductivities as high as 10^5 S cm^{-1} have been achieved, comparable to that of copper (10^6 S cm^{-1}).

High conductivity and processibility, both essential for industrial applications, were previously thought to be incompatible. But the addition of long, flexible chains — simple alkyl substituents (C_6–C_{20} chains) or ether- and amide-containing chains (4–14 atoms long) — to the monomer units before polymerization renders polythiophenes soluble in common organic solvents, and hence possible, in their conducting (doped) states or insulating (undoped) states. These soluble polymers (see 2*b* in the figure), like the parent polymer (2*a*), are highly coloured or black in the conducting state. Because transparency is associated with a small



1, Polyacetylene; 2, polythiophene if R is an H atom (*a*) or R can be a long, flexible chain (*b*); 3, polypyrrole; 4, poly-*para*-phenylene; 5, polythienylene-vinylene (R is H, *a*, or an alkoxy chain, *b*); 6, poly-*para*-phenylene-vinylene (R is H, *a*, or –O–C_6H_{13}, *b*).

excitation energy (band gap) for the promotion of electrons into the conducting state, transparent or colourless materials should also be good conductors. Only one polymer is known which is both transparent and conducting, poly(isothionaphthalene), but this material is not processible.

R. Elsenbaumer (Allied-Signal Inc.) noted that polythiophene derivatives in which the heterocyclic rings are linked through a vinyl group (5*a* in the figure) have smaller band gaps than the parent polymer (2*a*) in which the rings are linked directly. Substitution of strongly electron-donating alkoxy groups onto thiophene rings also reduces the band gap. By

* *International Conference on Science and Technology of Synthetic Metals*, Santa Fe, 26 June–2 July, 1988.