those of Levitt. Van Gunsteren *et al.* use the non-specific electrostatic and van der Waals' interaction function of Lifson for their hydrogen bonds. They attempt, however, to take account of the intermolecular contacts and solvent environment on the dynamics of a protein in the crystal in order to improve the agreement with the X-ray structure. Their simulation was carried out on a unit cell containing four protein molecules and 560 water molecules with the result that the time span was limited to a 20-ps trajectory. The structure of each molecule differs from the other three and from the X-ray structure, but the average over all four differs from the X-ray structure by only 1.2 Å r.m.s. for all atoms in the molecule.

All in all, results from computer simulation well justify Weber's<sup>20</sup> statement: "The protein molecule model resulting from the X-ray crystallographic observations is a 'platonic' protein, well removed in its perfection from the kicking and screaming 'stochastic' molecule that we infer must exist in solution".  $\Box$ 

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## Planetary science Magnetism and evolution of the terrestrial planets

## from J.A. Jacobs

A RECENT paper by David Stevenson and his colleagues<sup>1</sup> attempts to account for the properties (or absence) of intrinsic magnetic fields in the terrestrial planets — Earth, Mercury, Venus and Mars — in terms of their composition, internal structure and thermal history. Except in the case of Earth, where a large amount of seismic data is available, study of the intrinsic magnetic field provides one of the few clues to the nature of a planet's interior. Although Stevenson *et al.* cannot come to firm conclusions for all the planets, their analysis makes it possible to rule out a number of suggested models.

The Earth's magnetic field is predominantly dipolar (moment  $8 \times 10^{22}$  Am<sup>2</sup>), Mercury has a considerably smaller but nevertheless significant intrinsic magnetic field (dipole moment ~ 2.8-4.9 ×  $10^{19}$  Am<sup>2</sup>), whilst Venus and Mars have no, or at least extremely small, magnetic fields. The absence of a magnetic field on Venus, which is almost the same size as the Earth, cannot be because of its much slower rate of rotation (~ 243 days), since, as Hide<sup>2</sup> first pointed out, Coriolis effects are still dominant for any large-scale motions in the core.

It is generally accepted that the Earth's magnetic field is produced by dynamo action in the mainly iron fluid outer core, although there is not complete agreement on what drives the fluid motions. The most probable cause is either thermal convection or chemical buoyancy due to gravitational differentiation of the core into a solid heavier inner core and a lighter fluid outer core. The main advantage of chemically driven convection is its much greater thermodynamic efficiency. Indeed, convection driven by gravitational differentiation may occur even though the overall temperature gradient is sub-adiabatic<sup>3</sup>. In their analysis, Stevenson et al. assume that all the terrestrial planets underwent differentiation into a core and mantle and that any magnetic field is the result of dynamo action driven by thermal or chemical convection in a fluid core or fluid outer core.

If substantial radioactive heat sources are absent in the cores of the terrestrial planets, as is now generally believed to be the case, the paper shows that the heat flux from the cores due to secular cooling alone would probably now be sub-adiabatic and dynamo action would have ceased more than 1,000 Myr ago. On the other hand, if chemical buoyancy is the driving force for the fluid motions, then the existence or non-existence of a magnetic field depends on whether the planets possess solid inner cores.

The planets are described by a two-layer model with average densities and average heat capacities for mantle and core, and material parameters chosen so that present-day estimates of heat flux, uppermantle temperature and viscosity, and inner core radius are obtained for the Earth. Whole-mantle convection is assumed and any phase changes in the mantle neglected. The inner core is assumed to consist of pure iron, the outer core containing some light alloying component (sulphur or oxygen). Initially the whole core is super liquidus. As the planet cools, a solid inner core will begin to form when the liquidus temperature is reached at the centre; with further cooling the inner core grows at the expense of the outer core.

The validity of all the models does not depend on a precise knowledge of the melting curve of pure iron since they are adjusted to give the correct size of the inner core for the present Earth. Also, the beginning of inner core formation depends on the ability of the mantle to remove heat from the core and not on the details of the core liquidus. Small changes in model parameters can lead to completely fluid non-convecting cores, convecting fluid outer cores with inner core growth and almost completely solid cores with only a thin outer fluid shell.

In the case of the Earth, all models give growth of an inner core beginning after 2,300-3,000 Myr, quite late in the Earth's history. Since the Earth's magnetic field is at least 3,500 Myr old (ref.4), the driving mechanism of the geodynamo may have changed over geological time. Stevenson et al. suggest that initially the Earth's magnetic field was sustained by thermal convection. After inner core growth began (1,500-2,500 Myr ago), the release of gravitational energy became the dominant source for the geodynamo. The authors further suggest that this change in the energy source might be reflected in certain features of the geomagnetic field such as the frequency of polarity reversals.

The models for Venus admit all three possible evolutions. Since models with almost completely solid cores require implausibly small amounts of light alloying components, Stevenson et al. favour a completely fluid stably stratified core to explain the absence of a magnetic field on Venus. Two possible implications are that Venus once had an appreciable magnetic field driven by thermal convection which died ~ 1,500 Myr ago, and that Venus will eventually have a solid inner core which might cause the dynamo to start up again. The failure of some of the models of Venus to form an inner core, as do all Earth models, is mainly due to the lower central pressure of Venus (290 GPa compared with 360 GPa in the case of Earth).

The models for Mars also admit all three possible evolutions. Stevenson *et al.* again favour a completely fluid core since, apart from the absence of a substantial magnetic field, it is predicted for a cosmochemically plausible sulphur content of 15 per cent or more by weight. In all the models of Mercury, growth of a large solid inner core begins early in its history (after 250–600 Myr). The heat flux from the core becomes sub-adiabatic at different times for the models, but convection in a thin outer core (and hence a magnetic field) is still present in all models being maintained by chemical buoyancy.

Stevenson *et al.*'s analysis adds considerably to our knowledge of the terrestrial planets' possible constitution. Hide<sup>5</sup> had already shown how to locate the electrically conducting fluid core of a planet from external magnetic observations, although in the case of the Earth not so accurately as using seismic data. There is no doubt that magnetism will continue to play an ever increasing part in helping to unravel the deeper structure of the planets.

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