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CALCULATIONS OF ELECTRICAL TRANSPORT PROPERTIES OF LIQUID METALS AT HIGH PRESSURES

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It is shown how the usual nearly-free-electron model for the electrical resistivity of simple liquid metals can be extended to the case of liquid transition metals such as iron. A simple prescription is given for calculating the resistivity at different densities and temperatures. As an application and example of the method, calculations on liquid iron at different densities have

been carried out and the resistivity of molten iron in the Earth's outer core is estimated. The effects of alloying iron with other elements are also considered. The calculated conductivity of the outer core is well within the limit required for the dynamo model of the geomagnetic field and agrees well with some recent shock wave data.

1. Introduction

Over the last few years there has been considerable progress in understanding the electrical transport properties of liquid metals. A simple model for calculating the electrical resistivity and thermoelectric power was proposed by ZIMAN (1961). In this model the current in the liquid metal is carried by the "valence" or conduction electrons which are scattered by the disordered array of the ions or atoms. This scattering gives rise to the resistivity which can be calculated using a Boltzmann equation approach. Many calculations of the resistivity of "simple" liquid metals at normal pressures and temperatures have been carried out; see, for example, ASHCROFT and LEKNER (1966), FABER (1969) and EVANS (1970, 1971). The results of these calculations indicate that this simple nearly-free-electron (NFE) theory is capable of giving a good description of the magnitude of the resistivity, its temperature dependence and its behaviour on alloying. DICKEY *et al.* (1967) have calculated the resistivity of the liquid alkali metals at high pressures.

In the "simple" metals, i.e. those which are not noble or transition metals, the scattering properties of a single ion can be described using the pseudo or model potential technique. The basic idea behind this method is that of replacing the actual strong potential of the ion

by a weak potential in such a way that the ion retains the original *scattering* properties. This weak potential (the pseudo-potential) can then be used in the Born approximation in perturbative calculations of electronic properties HARRISON (1966).

In this paper, we indicate how the NFE model can be applied to non-simple metals and in particular to the transition metal iron where the pseudo-potential treatment is no longer valid. When iron atoms are brought together to form a metal, the atomic 3d levels are not completely destroyed but become virtual or resonant levels of the ionic potential (ZIMAN, 1971). This means that conduction electrons near the Fermi energy in iron are very strongly scattered by this potential. The energy at which the electron-ion scattering cross section is a maximum corresponds to the middle of the d band in metallic iron.

We calculate the resistivity of liquid iron at atmospheric pressure and close to its melting point and then evaluate the resistivity as a function of density with the aim of estimating the electrical conductivity σ of the Earth's outer core. The latter quantity is an important parameter in the dynamo model for the geomagnetic field. Several empirical values for σ have been proposed, most of them based on dubious extrapolations of known experimental data of one kind or another. We compare our calculated value of σ with some recent high-pressure shock-wave data and discuss effects of alloying iron with nickel and silicon.

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A preliminary account of the iron calculation was given by JAIN and EVANS (1972).

2. Outline of the theory

A derivation of the present model has been given by EVANS *et al.* (1971) and DREIRACH *et al.* (1972). The resistivity ρ can be written as:

$$\rho = \frac{3\pi\Omega_0}{e^2\hbar V_F^2} \int_0^1 4(q/2K_F)^3 a(q) |t(q/2K_F)|^2 d(q/2K_F), \quad (1)$$

where Ω_0 is the atomic volume of the liquid, V_F is the velocity of an electron at the Fermi energy, e is the electronic charge and q is a measure of the scattering angle for an electron on the Fermi sphere of radius K_F . The factor $(q/2K_F)^3$ arises from the usual momentum transfer factor $1 - \cos \theta$ in the Boltzmann equation result for the relaxation time. The distribution of the scatterers enters through $a(q)$, the liquid structure factor or interference function,

$$a(q) = N^{-1} \left| \sum_i \exp(iq \cdot \mathbf{R}_i) \right|^2, \quad (2)$$

where N is the number of ions and the average is over all ion sites \mathbf{R}_i in the liquid. This quantity can be measured directly in neutron or X-ray scattering experiments.

The scattering properties of a single site are introduced through the transition matrix $t(\mathbf{K}, \mathbf{K}')$ which gives the probability of an electron in a plane wave state $|\mathbf{K}\rangle$ being scattered into another state $|\mathbf{K}'\rangle$ of the same energy by a single scattering event. If the potential at any scattering centre is spherically symmetrical, then we can write

$$t(\mathbf{K}, \mathbf{K}') = \frac{-2\pi\hbar^3}{\Omega_0 m (2mE)^{\frac{1}{2}}} \times \sum_l (2l+1) \sin \eta_l(E) \exp(i\eta_l(E)) P_l(\cos \theta), \quad (3)$$

where η_l are the angular momentum phase shifts of this potential. Now t has the dimensions of energy and is normalised to the atomic volume, $q = |\mathbf{K} - \mathbf{K}'|$, and θ is the angle between \mathbf{K} and \mathbf{K}' . $P_l(\cos \theta)$ is the usual Legendre polynomial. The phase shifts are evaluated at the Fermi energy $E = E_F$ measured relative to the zero of energy E_{MTZ} in the liquid metal; m is the electron mass.

In transition metals, the d phase shift η_2 increases

rapidly with energy and passes through $\frac{1}{2}\pi$ at a "resonance" energy E_r . It is clear from eq. (3) that at this energy the scattering cross section $|t|^2$ is a maximum. In order to indicate how the resistivity depends on the form of the d phase shift we write:

$$\eta_2(E_F) = \arctan \left(\frac{\Gamma}{E_r - E_F} \right), \quad (4)$$

where Γ is the half-width of the resonance. This approximation for η_2 is good provided the Fermi energy E_F is close to E_r . If the s and p phase shifts are small, then only the d contribution is important in eq. (3). The integral in eq. (1) can then be evaluated (approximately) because the integral is heavily weighted towards backward scattering, i.e. $q \approx 2K_F$, and the resistivity has the form

$$\rho \approx \frac{30\pi^3\hbar^3}{m e^2\Omega_0} \frac{a(2K_F)}{K_F^2} \frac{\Gamma^2}{E_F(\Gamma^2 + (E_r - E_F)^2)}. \quad (5)$$

The resistivity depends strongly on the width of the resonance, the position of the Fermi energy relative to the resonance energy and the radius K_F of the Fermi sphere. We have taken the Fermi velocity V_F equal to $\hbar K_F/m$, the usual free-electron approximation. To make first-principles calculations of the resistivity, one needs the appropriate electron-ion potential, the Fermi energy in the metal, information about the liquid structure factor and a prescription for evaluating the Fermi radius K_F .

Although there are many approximations and assumptions inherent in this simple theory (see DREIRACH *et al.*, 1972), it does appear to give a good understanding of the electrical resistivity in liquid noble metals, iron, nickel and many alloys.

3. Details of the calculations

In order to evaluate the phase shifts which go into eq. (3) for the scattering amplitude, we need a method for constructing the electron-ion potential in a liquid metal. The method adopted in the present work was the so called "muffin-tin" model which is usually employed in energy band structure calculations in solids. A "muffin-tin" potential is one in which the potential is taken to be spherically symmetrical within a sphere of radius R_{MT} centred around a given atom (in the solid or liquid). Outside of this radius R_{MT} , the potential is set equal to a constant, E_{MTZ} . The radius R_{MT} is usually