integrated into the existing data networks, particularly the rapidly expanding Internet community.

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Earth's core

S. K. Saxena

The new techniques of heating solids with a laser at ultra high pressure in a diamond-anvil cell are providing us with new data on equation of state properties of solid and molten iron. The new data on iron melting, which extends to a pressure of nearly 2 megabar (200 GPa), permits the thermodynamic extrapolation of the melting data to pressures corresponding to the centre of the earth. The new studies on iron have also prompted a search for new phases of iron possible at high pressure and temperature. The currently available data point to a rather simple compositional model of the core which is identical to the meteorite irons or stony-irons. The adiabatic temperature of the earth's centre may lie between 5980 and 6680 K.

SEISMIC data show that the earth's core consists of an outer part which has all the properties of a liquid and an inner core which is solid (Figure 1). The core, reaching to a depth of nearly 2900 km from its centre stores a substantial part of the planet's energy and, therefore, exercises significant influence on the dynamic processes in the mantle. From cosmochemical, geophysical and geochemical considerations, the dominant species in the core has to be iron. Iron occurs in four solid structural states, namely, δ (bcc), α (bcc), γ (fcc) and ε (hcp). The ε (hcp) is considered to constitute the bulk of the solid inner core. Although not experimentally shown but based on the available data on the compressibility of iron (ε), it appears that iron by itself has a density higher than the density of the core[1]. Therefore, it has been suggested by many geochemists that some additional light elements (e.g. sulphur, oxygen, Si) are mixed with iron to form a lower density inner core and a lower melting liquid outer core[2].

To understand the state of the core, it is important that the thermodynamic properties of liquid and solid iron are determined. Recent developments in generating ultra-high pressures in diamond-anvil cells with laser heating have made it possible to study properties of material at the core pressures and temperatures. The purpose of this article is to report these technical developments, the recent findings on iron and the status of our understanding of the earth's core.

Figure 2 shows a summary of the currently available experimental data, until the year 1993, on phase equilibrium relations obtained from static devices, i.e. techniques with *in-situ* heating of a sample under pressure

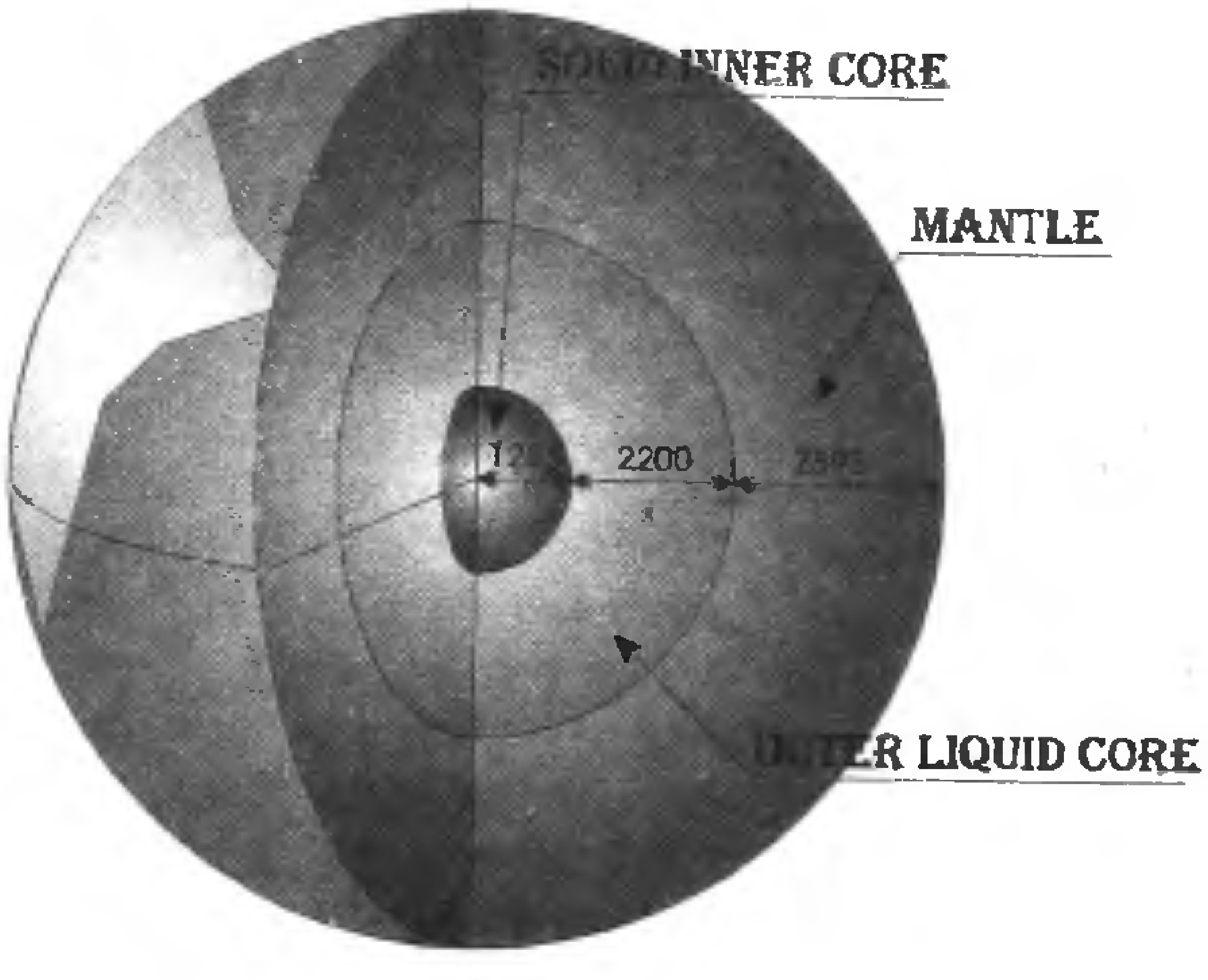

Figure 1. Earth's interior as determined by seismological data. The solid inner core with a radius of 1255 km is surrounded by a layer of molten iron with a shell thickness of ~ 2200 km reaching a depth of nearly 2900 km from the crust The inner core density is close to $13\ \mathrm{g\ cm^{-3}}$ and its temperature is variously estimated as between 4000 and 8000 K.

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sustained over a period of time. The phase transition boundaries α–γ, γ–ε and α–ε meet at one point, the so-called triple point; at such pressure and temperature all the three forms of iron coexist in equilibrium. Recent theoretical study on iron properties at high pressure and high temperature by Anderson[3] has shown that an experimental determination of the data on ε–γ phase transformation and the ε–γ-melt triple point are particularly crucial in extending our currently available results to understand the state of the earth's core. The argument is that the pressure-temperature of the triple point determines the behaviour of the melting curve at high pressures. Thermodynamically, the pressure-temperature slope of the ε–γ phase equilibrium curve constrains the estimated enthalpy, entropy and other physical properties of the ε phase which are largely unknown. With the availability of the equilibrium data on the ε–γ phase transformation, one may assess the thermodynamic properties of the ε phase which in turn can be used in the estimation of the properties of the iron melt.

A triple point, similar to the one shown in Figure 2, should exist for the coexisting γ, ε and melt. All the available experimental data on the ε–γ transition (see Figure 2), appear to indicate that such a triple point would lie around 2700 K between 60 and 70 GPa. The problem is that Brown and McQueen[4] had located a solid–solid transition some years ago at 4400 ± 300 K at a pressure of 200 ± 2 GPa. As shown in Figure 2, this phase transition could not be the ε–γ transition. The triple point is located at too low a pressure for this to be possible. This apparent inconsistency between the sets of data led Boehler[5] to conclude that there should exist a fifth iron phase. The existence of this phase is supposed to solve two problems; first it would explain the phase transformation recorded by Brown and McQueen in their shock-wave studies and second, by creating a third triple point, it would let the melting curve slope appropriately to fit the existing geophysical data. This led to the start of a search for a new phase of iron and the determination of the iron melting at pressures higher than that at the core/mantle boundary (130 GPa). Achieving such extreme pressures in the laboratory requires special techniques, for example, the laser heated diamond-anvil cell.

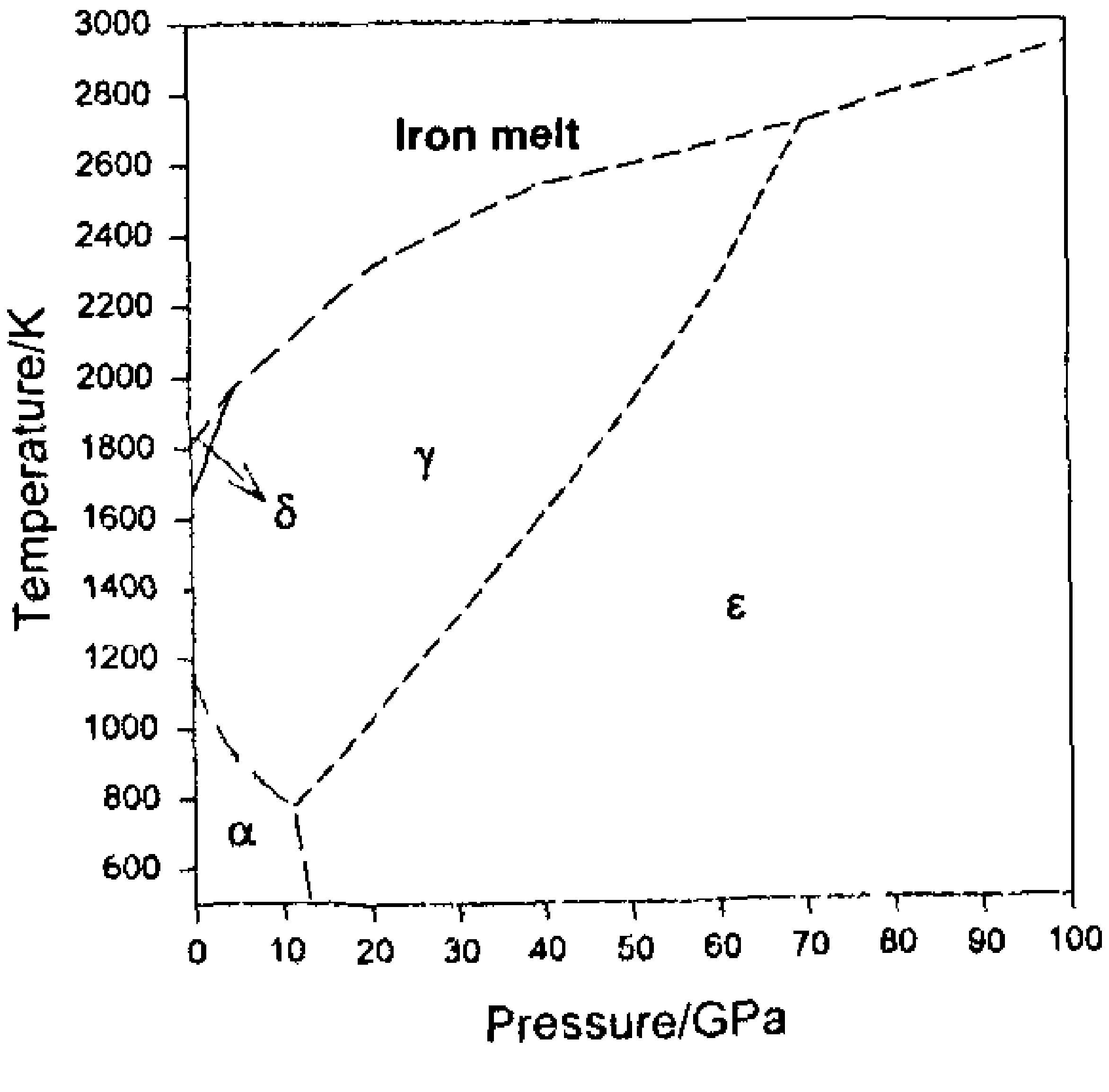

Figure 2. Phase diagram of iron from the available data up to 1993 The various curves drawn do not include the new experimental data The stability regions are shown for the four iron polymorphs δ (bcc), α (bcc), γ (fcc) and ε (hcp).

The diamond-anvil cell experimental set up for generating high pressure is discussed in several recent articles[6]. Here a brief description specific to Uppsala Laboratory is given (Figure 3). The laser heating system most useful for such studies is the one developed by Boehler *et al.*[7]. The use of a high power Nd : YAG laser (e.g. the one by Coherent) operating in CW TEM_{00} mode at a wavelength of 1064 nm is required. The laser provides maximally 35 W of vertically polarized light with a feedback controlled stability better than 0.5% peak-to-peak. The high pressure requires the megabar diamond anvil cell developed by Jephcoat *et al.*[8] for such experiments. To achieve real high pressures beyond 100 GPa, one needs to use the standard Drukker type IA beveled diamond anvils with 0.30 mm diameter flat culet faces (Figure 4). For the pressure determination the calibrated pressure shift of ruby R1 fluorescent line is used[8]. A phase transformation is determined by visual observation of melting when possible and by plotting the laser power against the temperature. At the temperature of phase transformation there is a distinct change in slope. The temperature is determined by spectroradiometry. The 50 μm in diameter slit of the

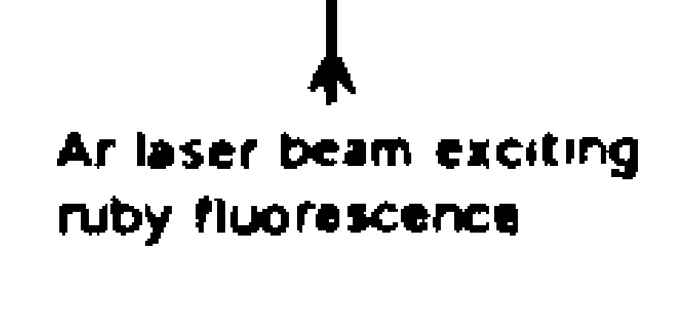

Figure 3. Experimental set up for the study of iron in a laser-heated diamond-anvil cell.

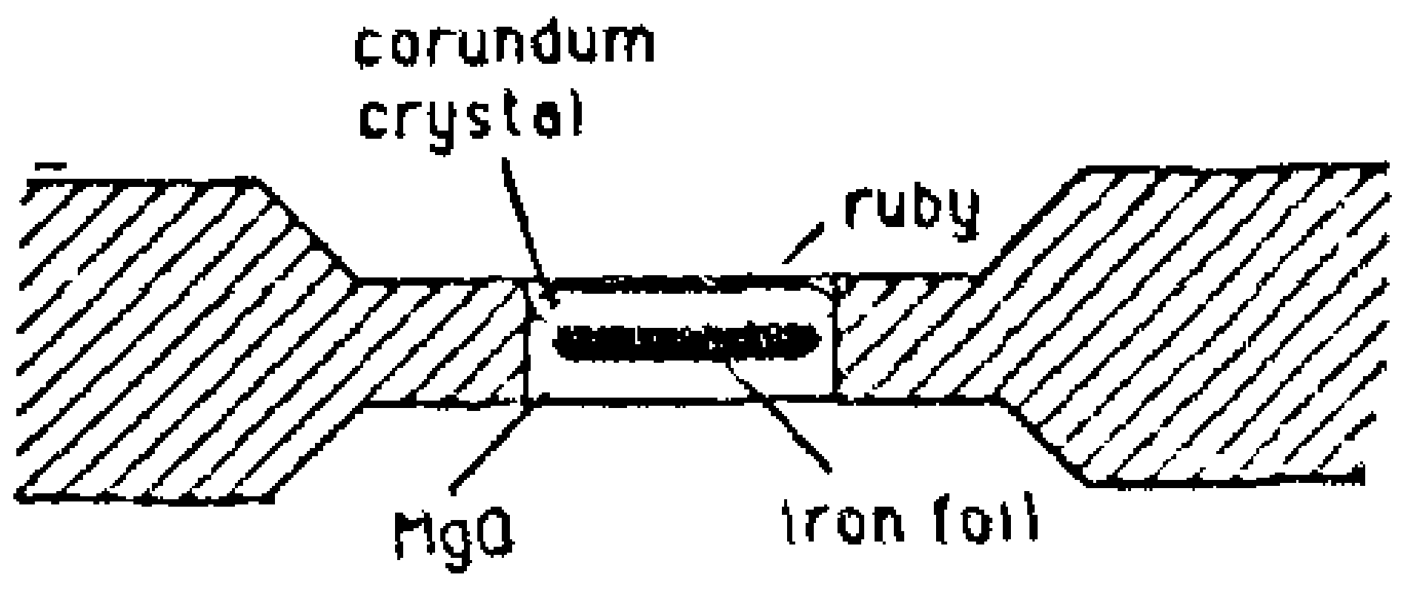

Figure 4. The sample environment in the experiment on melting The iron foil is cushioned with MgO powder with a corundum plate on the top. Ruby chips are used for pressure calibration

spectrograph collects the radiation from an area of 3 μm in width of the sample. A two-dimensional CCD detector is used to obtain temperatures measured over the entire length (30 μm) of the slit area. The temperature gradient over the central area (3 μm) is only a few degrees. The laser power fluctuations are minimized to a root mean square value < 0.5% by using a laser power stabilizer. In the method suggested by Boehler *et al.*[7] a ruby crystal is used on the top of the sample as an isolator and MgO powder at the bottom. The use of crystals eliminates the possibility of any significant reaction between the sample. In particular, at the subsolidus temperature range of such study, reaction between the iron and the ruby is not a problem. An area of 3 μm^2 is sampled by the spectrograph to get one pressure value; this reduces errors in pressure determination resulting from the presence of pressure gradient in the chamber. The pressure is determined at room temperature. Following the discussion by Heinz[9], a 7% decrease in the cold pressure may be made to account for the thermal pressure. Prior to measurement, a chosen spot is heated by laser to mechanically relax sample assemblage. The pressure usually drops up to 16% of the initial unrelaxed value. The pressure drop is almost linear and can be stabilized by repeated heating. The following problems are cited with the diamond-anvil cell experiments: i) reaction with the pressure medium and ii) temperature and pressure gradients. We dry the cell carefully. The corundum plate in contact with the iron does not show any visible reaction. Data on melting at high pressures show that corundum melts at higher temperature than iron at all pressures studied. We measure temperature over an area of less than 3 μm where melting was observed directly at lower pressures. It is further ascertained by the change in slope on a plot of the laser power against temperature. At high pressures (above 40 GPa) visual observations become difficult and then one must use the laser-power/temperature function and quench textures. Saxena *et al.*[10] demonstrated the accuracy of the temperature measurements by melting several solids with known melting temperatures.

In Figure 5 results of some recent experiments are displayed. The figure shows the stability of a new phase (called β by Saxena *et al.*[10]) and melting of iron to a pressure of 150 GPa by Saxena *et al.*[10]. Melting data are available to a pressure of nearly 200 GPa by Boehler[5]. The issue of the new phase is not fully resolved. It is likely that we have many additional structural modifications of iron. To begin with it is possible that the phase transformation reported by Boehler and Saxena *et al.* are for two different phases. In a recent study, by using the laser heated facilities at the Brookhaven National Laboratory synchrotron X-ray facilities, Saxena *et al.*[11] found that the hcp-iron (ε) transforms to a dhcp-iron (a four-layered hcp structure) at about 35 to 40 GPa at approximately 1500 K. This is certainly a confirmation of the possibility that we may have one or more yet unknown polymorphs of iron to be discovered.

Saxena *et al.*[10] used the new experimental data to obtain an internally consistent thermodynamic database with which to model the iron phase diagram and the core energetics. The newly generated data may then be used to calculate iron phase diagram. This combination of thermochemical and experimental data provides us with an estimation of temperature gradient in the earth's core.

Figure 6 shows the calculated phase transformations and melting in iron at pressures from 0 to 350 GPa. The extrapolation of the melting curve is done by calculating the melt compressibility as a function of temperature from the experimental data of Boehler and from this study (model 1). In such assessment of thermodynamic data, we did not include the nearly 10 to 15% error of pressure measurement possible when pressure exceeds 100 GPa (ref. 8). We generated a second model by permitting the melt compressibility to decrease at a higher rate at high temperatures by including the lower limits of the shock-wave data from Brown and McQueen[4] (see Figure 6). The high temperature melt data should be shifted to lower pressures by approximately 10%, which is quite within the stipulated random errors in the pressure measurements from the ruby fluorescence[8]. On such a melting curve (model 2), there are two triple points; the first (melt-β-γ) is located at 2946 (±100) K and 76.5 (±4) GPa; the second is located at 4580 K and 216 GPa insuring that the shock-wave constraint on melting[4] is satisfied. If we use the

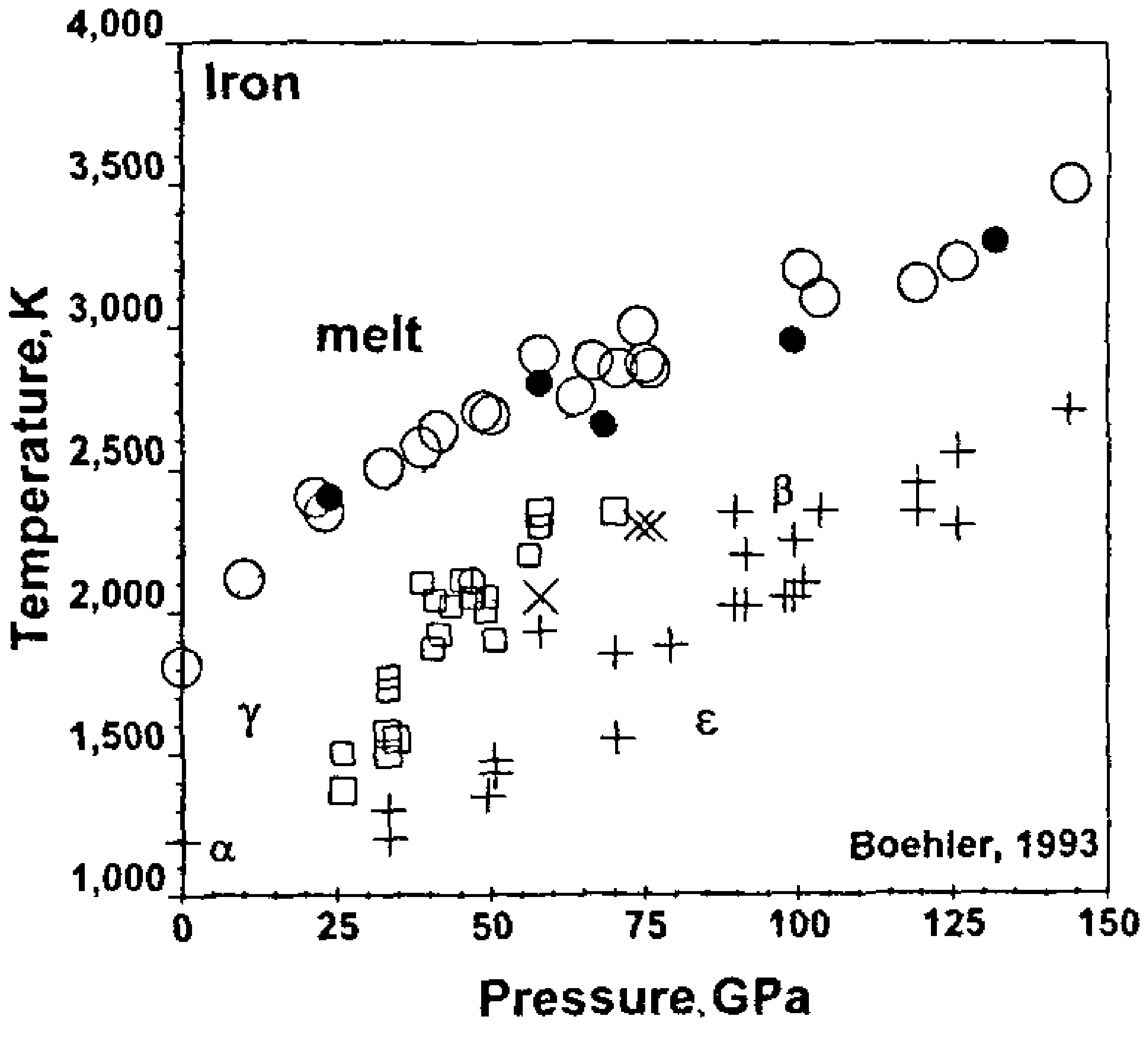

Figure 5. The experimental data on iron phase transformation and melting generated at Uppsala The open circles represent the melting temperature determined from either visual observation or using the laser-power/temperature slope change. The size of the circles represents the error in temperature due to laser fluctuation and statistical errors of fit The solid circles represent that iron remained solid up to that temperature. The squares represent the e–g transition and the plus sign the new phase β–ε transition. Crosses represent a phase transition which could not be labelled as either the β–γ or ε–γ

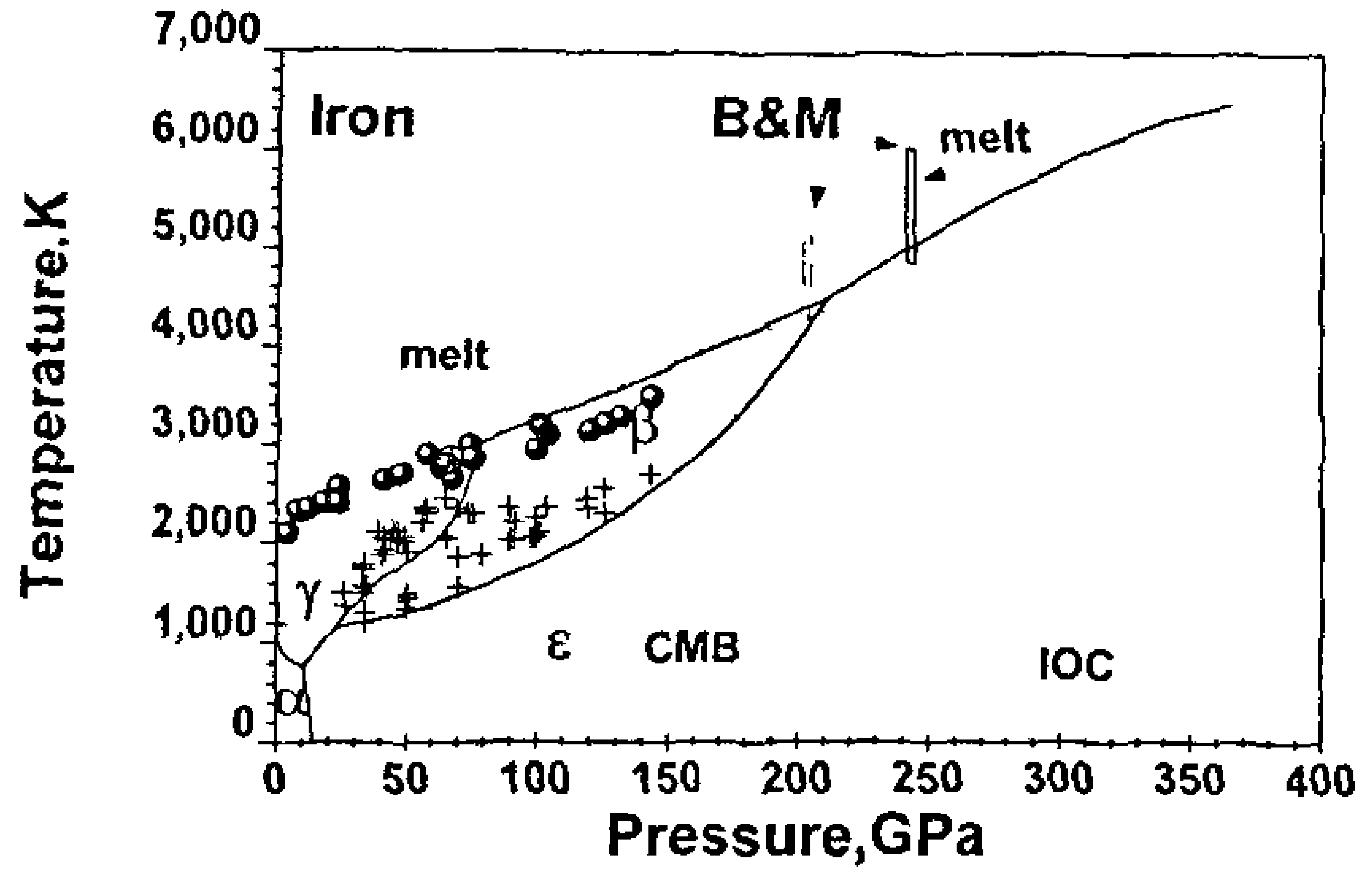

Figure 6. Iron phase diagram as calculated from the thermodynamic data from Saxena *et al*[11]. The dashed line represents an extrapolation of the melting curve (thermodynamically calculated) with no consideration of the data by Brown and McQueen[4] (labelled as B & M). The solid line represents the preferred model and includes the consideration of the latter data within the experimental errors of pressure determination.

low-temperature limits of these data as found through model 1 which gives the second triple-point (melt-β–ε) at 4015 K and 205 GPa.

A model of the earth's core should (a) explain why the inner core is solid and the outer core liquid, (b) must use a chemical composition which is consistent with cosmochemical data and (c) be similar in density to the seismic density. We note that the answer to the first problem lies in the special melting characteristics of iron associated with phase transformations and the location of the triple point ε–β-melt. The calculated melting curves in Figure 6 show that we may expect iron melting to occur at central core pressures (363.85 GPa, PREM model[12]) between 5980 (model 1) and 6680 K (model 2). Then if we assume that the temperature in the inner core is largely adiabatic, we may start the calculation of the adiabat starting where the pure iron melting curve intersects the inner-core/outer-core seismic discontinuity. The calculated temperature (model 2) at the earth's centre is 6150 K and at the top of the inner core 6130 K. The calculated densities of ε-iron just below the melting temperatures (13.76 g mol^{-1} at 5979 K and 13.55 g mol^{-1} at 6679 K) are considerably higher than the PREM model densities. Similar conclusions led Jephcoat and Olsen[1] to suggest that the inner-core must contain a few per cent of a light component such as pyrite. A light component both reduces the density and the iron-melting temperature. To maintain a solid inner core with the appropriate PREM densities, it is sufficient to add a small amount of Mg_2SiO_4 (high pressure equivalent phases: perovskite + periclase) to ε-iron (Figure 6). Both perovskite and periclase are refractory phases, with melting temperature higher than iron[13]. At the centre, the correct density is produced when we add 1.05% solids at 6150 K. In the inner core, it was not necessary to change the composition to obtain correct densities at slightly decreasing temperatures until the geotherm meets the inner/outer core boundary at 6133 K close to iron melting at 328.85 GPa. For the geothermal gradient to change smoothly and approach the outer core and mantle boundary at ~ 4000 K, the mole per cent of solids should increase from 0.7 at the bottom of the liquid core to 1.64 at the top. For a given composition, the outer core densities *do not change significantly with temperature. However*, a small decrease in the amount of added solid raises the temperature significantly. With model 1, we found the inner-core temperature to vary from 5430 to 5419 K and PREM density is matched with 1.5% of solids. A little additional amount of solids (~ 1.8%) is required to match the density in the outer-core along the thermal gradient shown in Figure 6. Although Anderson[14] used different thermodynamic arguments, his calculated temperatures of 6450 K for the centre and 6210 ± 400 K for the inner and outer core boundary are quite similar to the temperatures shown here. The second model is also in general agreement with the results of Brown and McQueen[4].

The experimental iron phase diagram and the thermodynamic data result in a rather simple model for the core. The relationship between the earth and meteorites has been discussed thoroughly in the literature. The class of meteorites called irons and stony-irons are considered to be debris from differentiated broken up planetary bodies. What the present results tell us is that this picture fits the model of the earth's core very well. Thus the core has simply the same composition as the irons and stony-irons. The density from such compositions fits the seismic density well. Dilution of iron by addition of sulphur or another light element is not essential. The outer core is liquid because of the phase transformations in iron and its melting behaviour.

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