tion from the insulating antiferromagnetic state to the metallic state and suggests the possibility of an intermediate metallic antiferromagnetic state. The limitations of their approach is that it involves many parameters, only treats the magnetic fluctuations in an average way, and does not predict superconductivity.

These findings show that the organics are worthy of more extensive study. Theoretical studies should focus on simplifying the model of Kino and Fukuyama and should take into account the magnetic fluctuations through techniques developed for the theory of cuprate superconductors. More experimental studies are needed to systematically characterize the unconventional properties of the metallic state.

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HIGH-PRESSURE GEOPHYSICS

Iron: Beta Phase Frays

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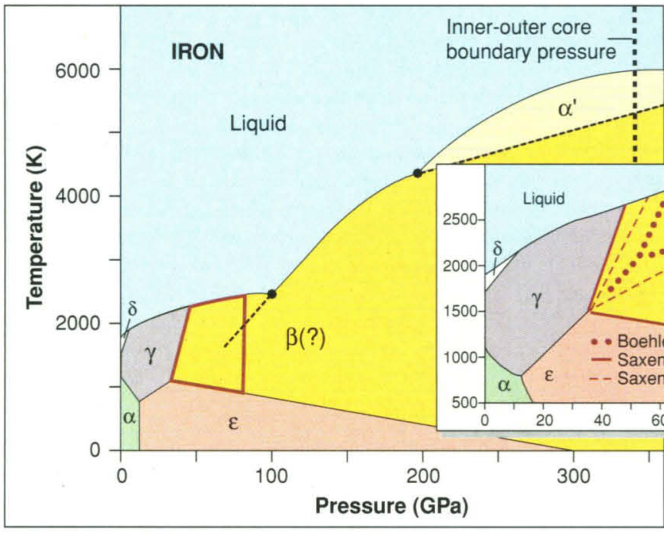
Geoscientists are interested in the properties of iron at high pressure in order to understand Earth's core, which is constituted almost entirely of iron. The phase diagram, a fundamental property of iron, has four accredited solid phases (α, γ, ε, and δ) mapped as high as 50.2 GPa and 2000 K (*1*) (see figure inset). Currently there is a dispute about whether the number of solid phases should be raised to five. Experimental data reported by Andrault *et al.* on page 831 of this issue (*2*) favor the validity of a fifth phase, called β, discovered and named by Saxena *et al.* (*3*, *4*). If authenticated, β would replace ε at the pressure and temperature conditions of Earth's inner core. The crystallographic structure of the inner core would change correspondingly, requiring a new look at theories of how Earth's core functions and affecting such fields as magnetogeodynamics, cosmochemistry, seismology, and first-principles calculations.



Iron's phases. The phase diagram of iron, which conforms to the latest melting temperature curve (*21*), upon which the proposed β phase (yellow) is placed. In the absence of β iron, ε iron, now hcp (hexagonal close packed) (pink) would extend to the high pressures and temperatures near Earth's core conditions. The region outlined in red shows where experiments testing for the presence of the β phase are currently done. (**Inset**) The boundaries for all established phases and three sets of boundaries for the proposed β phase. Phases: γ iron is fcc (face-centered cubic) (violet), α iron is bcc (magnetic body-centered cubic) (green), and δ iron is bcc (nonmagnetic body-centered cubic) (white). Another hypothetical iron phase, α′ (light yellow), is proposed to be bcc.

The fitful progress in discovering the complexities of the phase diagram of iron, characterized by contention followed by a big advance in experimental accuracy, exemplifies the aphorism of P. W. Bridgman, the patriarch of high-pressure physics: "... we never have perfectly clean-cut knowledge of anything, but all our experience is surrounded by a twilight zone, a penumbra of uncertainty.... the penumbra is to be penetrated by improving the accuracy of measurement." (*5*, pp. 33–34.)

In the late 1960s, a new experimental pressure device, the diamond-anvil cell, was developed. By the early 1990s, subsequent innovations allowed the temperature of experiments to be extended above 2000 K. This range permitted the determination of melting temperature T_m of iron at high pressure (above 50 GPa). Measurement of T_m was achieved by detecting a jump in a physical property such as electrical resistivity or optical reflectivity. The melting curve as a function of pressure *P* was measured to 43 GPa (*6*), then to 100 GPa (*7*), and finally to 197 GPa (*8*) at 3900 K by Boehler's group at Mainz. A competing measurement made by the Berkeley group (*9*) produced much higher values of $T_m(P)$, leading to a controversy over the temperature of Earth's core that lasted a decade. There was a standoff between the two groups because the measurement methods led to subjective conclusions about the value of T_m.

An absolute measure of the onset of the liquid state, showing where crystal structure diffraction patterns disappeared, was needed. X-ray diffraction arising from laboratory generators had been successfully used with the diamond-anvil cell, but at the high temperatures required for iron melting, the intensity of the diffracted lines weakened, giving inconclusive results.

When the diamond-anvil cell was attached to a terminus of a synchrotron beamline, the resulting intense x-rays provided high-quality, in situ diffraction patterns of iron structure even at quite high temperatures. Thus, the controversy about $T_m(P)$ was resolved in favor of the Mainz group, because the liquid structure of iron was found below the Berkeley melting curve and above the Mainz melting curve (*10*). The synchrotron radiation experiment described above was performed at the National Synchrotron Light Source at Brookhaven National Laboratories.

The diamond-anvil cell on the synchrotron beamline thus became a tool to explore

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the structural details of the iron phase diagram. Saxena *et al.* (the Uppsala group) claim to have found the structure of the β phase with use of this tool and reported it to be diagonal hexagonal close-packed (dhcp) (*4*). [Two years earlier, Boehler (*8*) had reported weak phase boundaries in the β region without measuring structure in the same year that Saxena *et al.* (*3*) reported phase boundaries without measuring structure]. Almost simultaneous with the dhcp announcement by the Uppsala group, Yoo *et al.* (*10*) reported that the structure of iron in the pressure and temperature region of concern was hcp (hexagonal close packed), not dhcp. And thus, the β-phase dispute was joined.

Contention over the proposed β phase has been strong in high-pressure meetings and in editorial correspondence for the last 3 years. The most detailed written description of the experimental issues involved can be found in two Technical Comments in *Science* (*11*). Most of the published reports pertaining to this dispute have been written by the Uppsala group, which is as it should be, because the burden of proof falls on those who propose a new phase. The opposition, the Livermore group and the Geophysical Lab group [the authors of (*10*)], maintain that the x-ray evidence for the dhcp structure in the β-phase region claimed by the Uppsala group could have other explanations. Further, they claim that their own research shows that the x-ray patterns in the disputed region (yellow portion of the figure) can be fully explained by the hcp structure.

Charges were made that the Uppsala group had not done enough experiments to validate their claim for a new structure. In response, the Uppsala group showed dhcp lines remained after the iron had been quenched from high temperatures (*12*), found dhcp lines in an in situ experiment (*13*), and determined enough reversible points to establish the slope of the γ-ε phase boundary (*14*) (see figure).

This series of experiments by the Uppsala group strongly supports their case. On the other hand, the long-standing reputation of the Geophysical Laboratory for research in this field means that their conclusion that hcp exists where Saxena *et al.* claim to find equilibrium dhcp cannot be dismissed. Dave Mao told the author (*15*) that "For samples of iron quenched after laser heating but remaining at high pressures, the geophysical lab repeatedly observed additional diffraction lines that could be interpreted as the dhcp phase. Since dhcp is not observed at simultaneous high P-T conditions by x-ray diffraction, this (evidence of dhcp) is interpreted as a quench product." The issue is whether dhcp exists as a phase in thermal equilibrium with fcc and hcp. Thus, we are faced with another standoff, the resolution of which requires improved accuracy of measurements, according to Bridgman's aphorism.

The diffraction patterns of the dhcp structure have all the lines of hcp plus two additional weaker lines. The solution probably lies in the detection and interpretation of weak diffracted lines and may also involve the resolution of closely spaced lines. The accuracy in the detection of weak diffraction lines and the resolution required to distinguish closely spaced lines are improved by the angle-dispersion method. Many believe that what is needed to resolve the dispute about the structure of the β phase is a synchrotron beamline of high brilliance (brilliance is defined as a high-intensity, small-focus beam).

The Brookhaven beamline has a lower brilliance than is required for angle-dispersion x-ray analysis of iron, so the experiments were done according to energy level (the energy-dispersive method). The requisite beam brilliance for the angle-dispersive method of measurement on iron is now available in the form of hard x-rays from a new generation of synchrotron radiation facilities, among which are the Advanced Proton Source (APS) at Argonne National Laboratory(*16*) and the European Synchrotron Radiation Facility (ESRF) in Grenoble, France (*17*). Angle-dispersive diffraction patterns for iron measured on dedicated high-pressure beamlines at these two facilities will likely give results definitive enough to resolve the present standoff.

However, William Bassett of Cornell University, who is associated with the Cornell High-Energy Synchrotron Source (CHESS) (*18*), cautions that perhaps not everything has been done to eliminate differences in experimental technique (such as rate of loading, deviatoric stress, and unpredictable properties due to sample setup).

Work with the angle-dispersion method is well under way. The Geophysical Lab group are undertaking their first experiment on iron at the APS facility. Andrault *et al.* announced the results of their first iron experiment at the Grenoble facility at the European Union of Geophysics meeting in March 1997. Although the French group verified the existence of the Uppsala group's β phase, they announced that its structure is orthorhombic, not dhcp.

Researchers from six laboratories (in Uppsala, Mainz, Livermore, Washington, D.C., Paris, and Lyon) in four countries are involved in the dispute over the existence of the β phase. Researchers from three of these laboratories (in Uppsala, Paris, and Lyon) are involved in the dispute over the exact structure of the β phase. Resolution of the conflicts may be close at hand, with new experiments at Argonne and Grenoble. These facilities have the latest, state-of-the-art technology; the brilliance of the beamlines in the hard x-ray region is thousands of times greater than earlier synchrotrons could muster (*16*). Another controversy looming ahead concerns the existence of the α′ phase above 200 GPa (see figure). The triple point at 200 GPa arises because there is evidence of a solid-solid boundary, found by measurements of sound velocity in conjunction with the shock-wave Hugoniot (*19*). The behavior of the sound velocity at 200 GPa (*19*) has been duplicated by molecular dynamics calculations, suggesting that the structure of the α′ phase is body-centered cubic (*20*). From data produced at the latest generation of synchrotron facilities, we may expect not only a critical evaluation of the β phase of iron, and perhaps of the α′ phase, but also unexpected directions of research. In the words of Arthur Bienenstock, Director of Stanford's Synchrotron Radiation Laboratory, "All our experience indicates that once you provide a significant [improvement] there will be new science that you just didn't anticipate at all" (*16*, p. 1906).

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