

Metallic Hydrogen at High Pressures and Temperatures in Jupiter**

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Abstract: Electrical conductivities of hydrogen were measured recently at 93–180 GPa (0.93–1.8 Mbar), 0.28–0.36 molcm⁻³, and 2000–4000 K. Shock temperatures were measured up to values of 5200 K at 0.83 Mbar. The conductivities indicate a continuous transition from a semiconducting to metallic fluid at 140 GPa and 3000 K. The results indicate that hydrogen becomes metallic much closer to the surface of Jupiter than thought previously and that Jupiter has no core–mantle boundary.

Keywords: high-pressure chemistry · high-temperature chemistry · hydrogen · Jupiter · metallic hydrogen

Knowledge of the properties of hydrogen at high pressures and temperatures is needed to understand the magnetic fields and the pressures, densities, and temperatures inside Jupiter and Saturn.^[1–3] The interiors are at high pressures and high temperatures because of the planets' large mass and low thermal conductivity. Pressure and temperature at the center of Jupiter are about 4 TPa and 20 000 K.^[3] Internal temperatures are well above the calculated melting curve of hydrogen.^[4] Properties of hydrogen must also be known to understand the interiors of new Jupiter-size planets now being discovered close to nearby stars.^[5] These giant planets might also be composed of massive amounts of hydrogen, since hydrogen has a cosmological abundance of approximately 90 atom %. For these reasons electrical conductivities and temperatures have been measured for fluid hydrogen and deuterium shock-compressed to pressures up to 180 GPa.^[6, 7] The conductivity experiments were performed with a reverberating shock wave to minimize the temperature and maximize pressure. The temperature measurements were performed at higher temperatures and lower pressures to investigate effects of molecular dissociation. The theoretical model for dissociation derived from the temperature measurements shows that the conductivity experiments probed primarily the molecular phase.^[6, 7]

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High shock pressures were generated by impact of a hypervelocity impactor onto the front surface of a sample holder containing liquid hydrogen.^[8] Al, Cu, or Ta impactors were accelerated to velocities up to 8 km s⁻¹ with a two-stage light-gas gun. Both hydrogen and deuterium were used to obtain different shock-compressed densities and temperatures. In the conductivity experiments hydrogen was contained between Al₂O₃ anvils, which in turn were contained between Al disks.^[6] Hydrogen shock pressure was determined by shock impedance matching the measured impactor velocity and known Hugoniot equations of state of the metal impactor, Al disk, and Al₂O₃ anvil. The pressure in hydrogen reverberates up to the first shock pressure in the Al₂O₃, independent of the equation of state of hydrogen.^[9] The reverberation of the shock in hydrogen between the Al₂O₃ anvils produces a relatively low final hydrogen temperature. The electrical resistance was measured, and the electrical resistivity obtained by calibration (conductivity is the reciprocal of resistivity). In the temperature experiments hydrogen was contained between an Al disk and an Al₂O₃ or LiF window.^[7] Pressure and density were obtained by shock impedance matching. The temperatures of the first shock and of this shock reflected off the window were determined by fitting the optical spectra of the emitted radiation to a grey-body spectrum.

At ambient pressure condensed molecular hydrogen is a wide bandgap insulator with $E_g = 15$ eV. Hydrogen is in the fluid phase in these experiments because the calculated temperatures are well above the calculated melting temperatures of approximately 1000 K at 100 GPa pressures.^[4] The shock-compression technique is very well suited for measuring the electrical conductivity of hydrogen because:

- 1) the high pressure reduces the energy gap,
- 2) the reverberating shock maintains temperatures at a few 0.1 eV, about 10 times lower than the temperature that would be achieved by a single shock to the same pressure,
- 3) the relatively low shock temperatures activate sufficient conduction electrons to produce measurable conductivities in the condensed phase,
- 4) electrode dimensions and separations are of the order millimeters, which are straightforward to assemble,
- 5) thermal equilibrium is obtained in a time less than the resolution (≈ 1 ns) of the measurements,
- 6) most importantly, the experiments are sufficiently fast (≈ 100 ns) that the hydrogen sample at high temperature cannot diffuse away.

The thickness of the hydrogen layer decreases from the initial value of 500 μm down to the compressed value of approximately 60 μm . Current flow reaches its equilibrium flow pattern in about 1 ns for a layer 60 μm thick with our observed minimum electrical resistivity of $5 \times 10^{-4} \Omega\text{cm}$. Supplemental experiments examining the electrical conductivity of shock-compressed Al_2O_3 show that the conductivity of hydrogen at metalization (140 GPa) is five orders of magnitude greater than that of Al_2O_3 .^[10]

The electrical resistivities decrease from about 1 Ωcm at 93 GPa to $5 \times 10^{-4} \Omega\text{cm}$ at 140 GPa and are constant at $5 \times 10^{-4} \Omega\text{cm}$ at 155 and 180 GPa, as shown in Figure 1.^[6] The

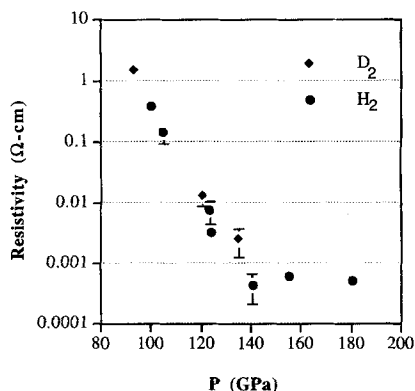


Figure 1. Electrical resistivity versus pressure for fluid hydrogen and deuterium. The saturation resistivity of 500 $\mu\Omega\text{cm}$ above 140 GPa is that of the metallic fluid (ref. [6]).

change in slope is indicative of the transition to the metallic state. Since our previous data^[11] show that the electrical conductivity of hydrogen is thermally activated, we analyzed these results in the range 93–135 GPa using our previous dependence for a fluid semiconductor [Eq. (1)], where σ is electrical

$$\sigma = \sigma_0 \exp(-E_g/2k_B T) \quad (1)$$

conductivity, σ_0 depends on density ρ , $E_g(\rho)$ is the density-dependent mobility gap in the electronic density of states of the fluid, k_B is Boltzmann's constant, and T is temperature.

The density and temperature were calculated by computationally simulating each experiment with a standard equation of state of hydrogen. Our least-squares fit of Equation (1) to the data gives $E_g(\rho) = 0.905 - (67.7)(\rho - 0.3)$, where $E_g(\rho)$ is in eV, ρ is in molcm^{-3} ($0.28 - 0.31 \text{ molcm}^{-3}$), and $\sigma_0 = 140 (\Omega\text{cm})^{-1}$. A value of $\sigma_0 \approx 200 - 300 (\Omega\text{cm})^{-1}$ is typical of liquid semiconductors.^[12] $E_g(\rho)$ derived from this fitting procedure and $k_B T$ are equal at a temperature of 0.3 eV and a density of 0.31 molcm^{-3} . In this region of density and temperature, the energy gap is smeared out thermally, activation of electronic carriers is complete, disorder is already saturated in the fluid, and conductivity is expected to be weakly sensitive to further increases in pressure and temperature. At 0.31 molcm^{-3} the calculated pressure is 120 GPa, which is close to the 140 GPa pressure at which the slope changes in the electrical resistivity. At higher pressures of 155 and 180 GPa the resistivity is essentially constant at $5 \times 10^{-4} \Omega\text{cm}$, a value typical for liquid metals. Thus, fluid hydrogen becomes metallic at about

140 GPa and 3000 K after a continuous transition from a semiconducting to metallic fluid.

As first noted by Hensel and Edwards,^[13] the electrical conductivity of fluid metallic hydrogen is essentially identical to that of fluid Cs and Rb undergoing the same transition from the semiconducting to metallic state.^[13]

About 5% of the hydrogen molecules are dissociated at metalization in the fluid at 3000 K (discussed below). The sizes of the hydrogen molecule and atom and their initial electronic energy gaps are similar; this suggests that in the mixed-phase fluid at high temperatures the two are mutually soluble and form a common mobility gap in their electronic density of states, so that the energy gap measured is that of the mixture.

The metalization pressure of 140 GPa in the warm fluid is substantially lower than 300 GPa, the typical theoretical value for the crystalline solid at 0 K.^[14,15] The lower metalization pressure in the fluid is probably caused by the fact that hydrogen molecules approach closer to one another in the warm disordered fluid than in the cold crystal. Also, the electronic energy gap is known to be very structure dependent,^[16,17] and the disorder allows the fluid to effectively sample many crystalline structures with lower band gaps. In addition several interactions occur in a cold lattice occupied by diatomic hydrogen molecules, which have a high zero-point vibrational energy, which can change crystal structure, orient their molecular axes relative to the crystal structure, and undergo charge transfer. These interactions in the crystal inhibit band-gap closure^[18] and are eliminated by melting, which thus reduces the metalization pressure relative to that of the solid.

We have also measured temperatures of liquid deuterium and hydrogen shock-compressed up to 83 GPa and 5200 K.^[7] The first-shock temperatures up to 20 GPa are in excellent agreement with predictions based on molecular hydrogen.^[19] The second-shock temperatures at pressures up to 83 GPa, obtained by reflection of the first shock off a window, are lower than predicted for the molecular phase. The lower measured temperatures are caused by a continuous dissociative phase transition above 20 GPa. This partial dissociation from the molecular to the monatomic phase absorbs energy, which causes lower temperatures than expected if all the hydrogen were to remain molecular. The theoretical model for molecular dissociation derived from the temperature data was used to calculate the dissociation fraction in the conductivity experiments.^[6,7] At 140 GPa and 3000 K the dissociation fraction is calculated to be about 5%. Since only about 5% of the hydrogen molecules are dissociated at metalization, electronic conduction is probably caused by electrons delocalized from H_2^+ ions.^[20] This is different than the monatomic phase predicted initially by Wigner and Huntington.^[21] However, the nature of hydrogen at these extreme densities is still to be elucidated.

Because hydrogen is in equilibrium in these experiments, the results were used to develop a theoretical model with which to calculate conditions inside Jupiter. Since Jupiter is approximately 90 atom % hydrogen, this simple approach gives important general features of the equation of state and electrical conductivity of Jupiter.

The shock temperature data were used to derive a model for molecular dissociation at high pressures and temperatures. This model was used to calculate the isentrope of hydrogen starting

from the surface conditions of Jupiter (165 K and 1 bar).^[22] When plotted as temperature versus pressure, the isentrope of hydrogen increases monotonically up to about 40 GPa, at which point the temperature reaches a broad plateau. The temperature of hydrogen might even decrease by approximately 2% from 40 to 180 GPa, as shown in Figure 2. This weak temperature de-

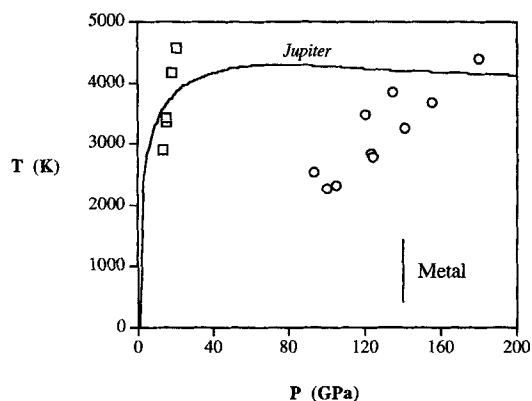


Figure 2. The solid curve is the isentrope of hydrogen calculated from surface conditions of Jupiter (165 K and 1 bar) plotted as temperature versus pressure. Open circles and squares are temperature and pressure at which electrical conductivities were measured (ref. [6] and [11]). Metalization of hydrogen in Jupiter occurs at 140 GPa.

pendence is caused by the continual increase in molecular dissociation with increasing pressure. Jupiter also contains approximately 10 atom % He. He is much hotter at a given density and pressure than is molecular hydrogen, because He has no internal degrees of freedom to absorb energy in this regime. Thus, the warmer He probably causes the temperature of Jupiter to always increase monotonically with increasing pressure, the condition that drives convection. Jupiter is known to be convective because it has a large external magnetic field produced by the convective motion of electrically conducting hydrogen by dynamo action. In addition, convective heat transfer to the surface is the reason why Jupiter radiates more internal energy than it receives from the sun. It is possible, however, that Jupiter is convectively quiescent over a radially thin region. A possible maximum in temperature versus pressure might induce an additional layer in the molecular region, as has been predicted to occur at 42 GPa by Zharkov and Gudkova.^[3] That is, a quiescent boundary layer over a long period of time might facilitate settling of ice and rock from hydrogen and cause an abrupt density change.^[22]

The continuous dissociative phase transition from the molecular to the monatomic phase means that there probably is no sharp boundary between the molecular mantle and the monatomic metallic-hydrogen core of Jupiter. Most recent models of Jupiter assume a sharp boundary between a molecular mantle and monatomic core at an internal pressure of 300 GPa.

A major issue about Jupiter is the region in which the magnetic field is produced. On the basis of calculations of electrical conductivities of dense fluid hydrogen,^[23–25] the magnetic field has been thought to be produced primarily in the monatomic metallic core and in the molecular mantle, as well.^[26–28] However, the relative contributions of each region have been uncer-

tain. The electrical conductivity inside Jupiter was calculated by evaluating Equation (1) along the isentrope of hydrogen described above.^[29] To demonstrate that electrical conductivities were measured at pressures and temperatures representative of those in Jupiter, both this hydrogen isentrope and the temperatures and pressures achieved in the electrical conductivity measurements are plotted in Figure 2.

The density-dependant energy gap was taken as the linear fit to the previous determinations.^[6, 11] The fit to these two data sets is given by Equation (2) in the range $0.13 < \rho < 0.3 \text{ mol cm}^{-3}$ with E_g in eV. The prefactors σ_0 determined in

$$E_g = 20.3 - 64.7\rho \quad (2)$$

the two sets of experiments differ by 10^4 at densities of 0.13 and 0.30 mol cm^{-3} . Values of σ_0 at intermediate densities were obtained by exponential interpolation of these data [Eq. (3)].

$$\sigma_0(\rho) = 3.4 \times 10^8 \exp(-44\rho) \quad (3)$$

Equation (3) fits the value of σ_0 determined at 0.13 mol cm^{-3} ($1.1 \times 10^6 (\Omega \text{ cm})^{-1}$), and σ_0 is close to the value obtained near 0.3 mol cm^{-3} ($1.4 \times 10^2 (\Omega \text{ cm})^{-1}$), where hydrogen is undergoing a continuous transition from a semiconducting to metallic fluid. Also, σ extrapolates to the metallic value of $\sigma = 2000 (\Omega \text{ cm})^{-1}$ (resistivity = $5 \times 10^{-4} \Omega \text{ cm}$) at 140 GPa.

The electrical conductivity of monatomic metallic hydrogen was predicted theoretically to be higher, $1-2 \times 10^5 (\Omega \text{ cm})^{-1}$,^[24] than measured for the molecular phase, $2 \times 10^3 (\Omega \text{ cm})^{-1}$ at 0.31 mol cm^{-3} and 3000 K.^[6] The metallic hydrogen conductivity predicted theoretically is expected to be accurate at higher pressures for densities above 0.5 mol cm^{-3} , where the molecules are expected to be fully dissociated into a monatomic metallic fluid. The electrical conductivity of hydrogen along the isentrope in Figure 2 is shown in Figure 3. The conductivity was calculated up to 120 GPa, where the electronic energy gap approaches the temperature, and was then extrapolated up to the metallic value of $2000 (\Omega \text{ cm})^{-1}$ at 140 GPa.

For comparison, we also calculated electrical conductivities in the molecular envelop of Jupiter^[26] using Equation (1) with $\sigma_0 = 300 (\Omega \text{ cm})^{-1}$, a value typical of a liquid semiconduc-

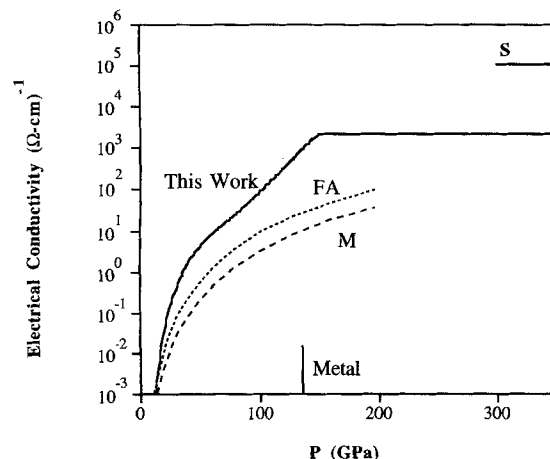


Figure 3. Electrical conductivities of hydrogen in Jupiter plotted versus pressure along isentropes of hydrogen. FA, M, and S are defined in the text (ref. [29]).

tor,^[12] and different relations of $E_g(\rho)$ at 0 K for molecular hydrogen calculated by Freidli and Ashcroft (FA)^[30] and by Min et al. (M)^[31], along an isentrope of hydrogen calculated by Saumon et al.^[32] These two curves, FA and M in Figure 3, can only be calculated up to 200 GPa where the temperature on the isentrope is equal to the bandgap of the molecular phase. As shown in Figure 3, for pressures below 20 GPa all three models approach a common value. For pressures above 40 GPa our calculated conductivities are one to two orders of magnitude greater than those calculated with FA and M. Further theoretical results^[24] imply that the conductivity of monatomic metallic hydrogen at what was thought to be the core–mantle boundary (300 GPa, 0.65 molcm⁻³, and 10000 K) should be 10⁵ (Ωcm)⁻¹ (S in Figure 3).

The metalization pressure of 140 GPa observed in the fluid^[6] is substantially lower than 300 GPa, the typical theoretical value for the solid at 0 K.^[14, 15] This lower pressure implies that hydrogen in Jupiter becomes metallic at about 0.9 of the radius, as predicted by Smoluchowski,^[27] rather than about 0.8 of the radius for 300 GPa. Because of the large volume of Jupiter this corresponds to about 50 more Earth masses of metallic hydrogen than thought previously. Also, an electrical conductivity as low as 20 (Ωcm)⁻¹ might contribute to the magnetic field of Jupiter because a conductivity of this value is thought to be responsible for producing the magnetic fields of Uranus and Neptune.^[33] As shown in Figure 3, a conductivity of 20 (Ωcm)⁻¹ is achieved in Jupiter at 80 GPa. For these reasons, the external magnetic field of Jupiter would be produced in the molecular envelop substantially closer to the surface with a metallic conductivity about two orders of magnitude smaller than thought previously.

The above results imply that the magnetic field of Jupiter is produced in the region in which fluid molecular hydrogen undergoes a continuous dissociative phase transition. Based on the theoretical model for molecular dissociation derived from shock temperature experiments, about 10% of the hydrogen molecules are dissociated at metalization in Jupiter (140 GPa and 4000 K). Once hydrogen metalizes, additional changes in electrical conductivity caused by the continuous molecular transition to complete dissociation at higher pressures are expected to be relatively small for an additional two- to threefold increase in pressure. That is, in a fluid the increase in the electrical conductivity is dominated by the increase in the number of conduction electrons. Once they are all excited to form a metal, further changes in conductivity are expected to be relatively small (factor ≈ 2) as density and temperature increase somewhat with in-

crease in pressure and depth, so that up to 2–3 times the observed metalization pressure, the electrical conductivity is about 2000 (Ωcm)⁻¹. At higher pressures, temperatures, and depths at which molecular dissociation becomes complete, the pure monatomic phase is expected to form a metallic plasma and the higher predicted conductivity is expected to apply. However, the external magnetic field is caused primarily by a conductivity of about 2000 (Ωcm)⁻¹ in the outermost portion of Jupiter.

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