

Conf. 810827-15

UCRL-86481
PREPRINT

DISCLAIMER

This report was prepared at a cost of \$20,000 by an agency of the United States Government. It is the property of the United States Government and is loaned to your agency; it and its contents, except those parts which are specifically granted to your agency, are to be held in confidence. It is not to be distributed outside your agency without the express written consent of the agency which prepared it. It is the property of the United States Government and is loaned to your agency; it and its contents, except those parts which are specifically granted to your agency, are to be held in confidence. It is not to be distributed outside your agency without the express written consent of the agency which prepared it. References here to any specific individual, business, or entity, or to any specific action, product, or process described or recommended in this report does not imply that such individual, business, or entity, or product, or process is necessarily a better choice than any other individual, business, or entity, or product, or process that may be available. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

SHOCK-WAVE STUDIES: MODELING THE GIANT PLANETS

UCRL-86481

DE82 016768

Marvin Ross
University of California
Lawrence Livermore National Laboratory
Livermore, California 94550

This paper was prepared for submittal to:

8th AIRAPT & 19th EHPRG Conference
Uppsala, Sweden
August 17-22, 1981

July 20, 1981

MASTER

Lawrence
Livermore
Laboratory

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

8b
DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

SHOCK-WAVE STUDIES: MODELING THE GIANT PLANETS

18452
Marvin Ross

University of California, Lawrence Livermore National Laboratory
Livermore, California 94550

ABSTRACT

The giant planets--Jupiter, Saturn, Uranus, and Neptune--differ markedly from the inner, or terrestrial, planets. Observations of their average density, gravitational moments, and atmospheric composition have enabled astrophysicists to draw some conclusions as to their structure, but efforts have been hampered by a lack of accurate data on the chemical, physical, and thermodynamic properties of constituent materials at the extremely high temperatures and pressures characteristic of planetary interiors. Shock-wave experiments conducted recently at LLNL have provided more accurate equations of state and electrical conductivities for many of these materials, and these have led to improved structural models of the giant planets.

INTRODUCTION

The recent flights of Pioneer and Voyager to Jupiter and Saturn, as well as anticipated visits to Uranus and Neptune, have stimulated a renewed interest in the structure of these giant planets. To construct accurate models, we must explain their observed luminosity, radius, oblateness, rotation rate, and gravitational moments in terms of equations of state for the postulated constituent materials. The simplest theory linking equations of state to structure is the static model which assumes the planets are in hydrostatic equilibrium and the temperature gradient is isentropic.

On the basis of recent calculations the giant planets are currently thought^{1,2} to consist of three layers: an outer layer of molecular hydrogen and helium; a middle layer either of metallic hydrogen and helium (for Jupiter and Saturn) or of icy ammonia, methane, and water (for Uranus and Neptune)²; and a rocky core of iron, nickel, silicon, and magnesium oxides. Hydrogen and helium are subjected to a very wide range of pressures and temperatures. From 1 bar and 160 K at the surface of Jupiter to 45 Mbar and 20000 K at the rock core boundary. The conditions in the ices are believed to range from 0.2 Mbar and 2200 K to 6 Mbar and 7000 K. The rocky core components are subjected to roughly 10 Mbar in Uranus and Neptune and to as much as 100 Mbar at Jupiter's center.

Most of the recent shock-wave data used to model the giant planets were obtained with the LLNL two-stage gas gun.³ This device can accelerate a 20-g metal projectile against a target at velocities up to 7 km/s. To achieve conditions comparable to those in the planetary interiors, H₂, CH₄, NH₃, and H₂O must be shocked from the liquid phase. All except H₂O have boiling points below room temperature, and thus the targets are actually small cryostats.

THERMODYNAMIC PROPERTIES OF HYDROGEN

There have been a number of static high pressure measurements on the thermodynamic properties of hydrogen and deuterium. These measurements include 4 K solid isotherms to 25 kbar,⁴ fluid isotherms to 300 K and 20 kbar,⁵ and melting curves to 57 kbar at room temperature.⁶ Nellis and Mitchell⁷ recently conducted single shock-wave experiments on liquid deuterium that obtained pressures up to 0.20 Mbar and that reached 0.80 Mbar and 7000 K. In addition, they plan more reflected-shock experiments at intermediate pressures.

To illustrate the significance of these shock-wave data to planetary modeling, we have compared pressure-temperature plots for computed isentropes of the current models of Jupiter and Saturn with our shock-wave results (Fig. 1). The shock Hugonots closely follow the paths of the planetary isentropes. In principle, we should be able to calculate the forces acting between hydrogen molecules. As an alternative to theoretical rigor we can determine an effective intermolecular potential which, when used with statistical mechanical models, will reproduce experimental data. These models can then be used to obtain a comprehensive equation of state over the range of pressure-temperature conditions in the giant planets. We started with the intermolecular potential of Silvera and Goldman⁸ who used a very accurate theory for molecular solids to determine a hydrogen pair potential that fits the solid (4 K) hydrogen and deuterium data to 25 kbar. We tested their intermolecular potential with an accurate theory for compressed hydrogen fluid and were able to predict the experimental fluid isotherms from 0 to 20 kbar and from 75 to 300 K, as well as the hydrogen melting curve to 54 kbar. To calculate hydrogen Hugoniot data, we modified the Silvera-Goldman potential at small intermolecular separations. The high temperatures accompanying the shock process makes the shock-wave data very sensitive to the short range repulsive forces. Their potential had been fitted to low-temperature solid-hydrogen data below 25 kbar, and does not extrapolate correctly beyond that region. The new potential now fits all the condensed hydrogen data from 1 bar to about 0.80 Mbar and 7000 K.

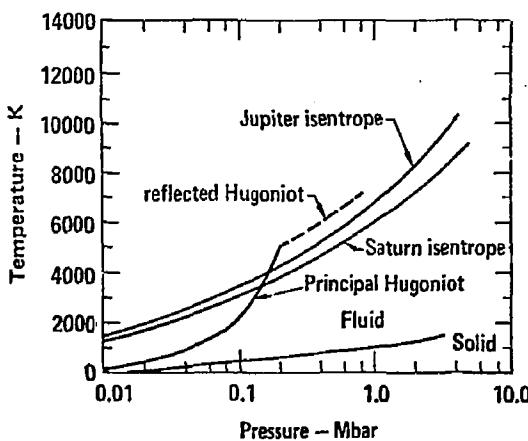


Fig. 1 Comparison of our experimental shock-wave results with the isentropes for Jupiter and Saturn.

THERMODYNAMIC PROPERTIES OF HELIUM

Very recently the equation of state⁹ of fluid helium-4 has been measured up to 20 kbar. The room temperature melting point¹⁰ near 120 kbar has also been determined. Together with earlier work¹¹ on the equation of state of the 4 K solid to 20 kbar, these recent measurements provide a set of thermodynamic data suitable for testing statistical mechanical theories of molecular solids and fluids. At the present time there is no shock-wave data for liquid helium. To extend these experimental data to high pressure, we have made electron band structure calculations to 200 Mbar.¹² We found that helium should become metallic at 112 Mbar and thus behaves as an insulator in planetary interiors. We have employed the lattice dynamics and liquid perturbation theories used to calculate accurate thermodynamic properties for H₂ and D₂ to determine a pair potential for helium sufficiently accurate to generate thermodynamic data in good agreement with experiment to 120 kbar. We extended the pair potential to very high pressures by also requiring it to fit the equation of state predicted by electron band theory. In this way we have developed a theory of condensed helium that can be used to predict thermodynamic properties over the whole range of interest. Using this potential we calculated the liquid Hugoniot shown in Fig. 2. The temperature of 20000 K calculated at the highest pressure is comparable to the maximum temperature in the hydrogen-helium layer of Jupiter and exceeds that in Saturn (11000 K). Shock wave experiments are being planned to test the theory.

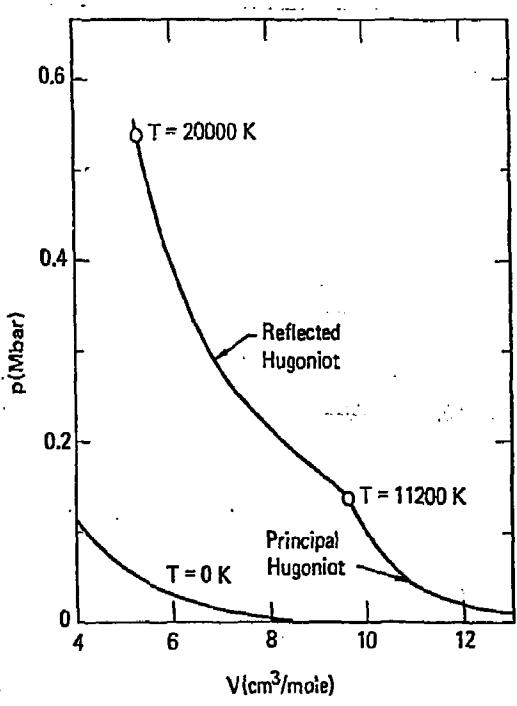


Fig. 2 Predicted principal and reflected Hugoniots for liquid helium.

Using equations of state based on hydrogen shock-wave experiments, the internal structure of Jupiter can be modeled in such a way as to explain all of its observed properties, while retaining the same proportions of constituent elements as existed in the sun when it was formed. Saturn on the other hand emits as much as 2.5 to 3 times the heat of its solar input. Stevenson¹³ has suggested that at the lower Saturn temperatures helium and metallic-hydrogen separate and the excess energy is the result of gravitational separation. This then results in a surface depletion of helium, a fact that appears to be confirmed by the recent Voyager 1 flyby of Saturn. Improved thermodynamic and solubility calculations of helium-hydrogen mixtures with additional input from shock-wave experiments may assist in providing additional understanding.

THE ICES (H_2O , CH_4 , NH_3)

The middle "ice" layer of Uranus and Neptune is believed to consist mainly of fluid, H_2O , CH_4 , NH_3 of solar composition.² The estimated pressures and temperatures of the "ice" layer ranges from about 6 Mbar and 7000 K at the inner core/ice boundary, to about 0.2 Mbar and 2200 K at the outer ice/hydrogen-helium boundary. Our recent shockwave experiments on these liquids,¹⁴ as well as theoretical studies,¹⁵ imply that the H_2O and NH_3 in the "ice" layer are almost totally ionized and the CH_4 has been pyrolyzed to carbon.

Figure 3 compares some of this data for the "ices" with an isentrope calculated for Uranus (Neptune is very similar). The figure demonstrates the significance of the data to theoretical modeling studies of these planets. For methane the experimental

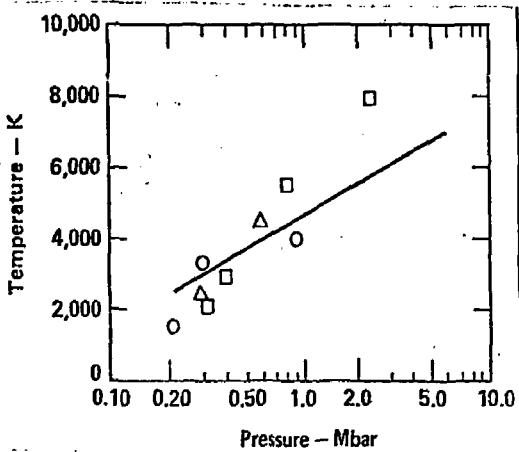


Fig. 3 Plot of some experimental shock-wave data for water, ammonia, and methane in the range of temperatures and pressures predicted in the Uranus (and Neptune) "ice" layer. Note the pressure scale is logarithmic.

data, only some of which is shown, consists of a principal Hugoniot up to 0.45 Mbar, plus one data point reflected from 0.23 Mbar to 0.91 Mbar. A careful inspection of the shock data and chemical equilibria calculations for the dense fluid predict that above 0.20 Mbar and 2000 K, methane is converted into elemental carbon and molecular hydrogen. Recent theoretical calculations on Hugoniots of many hydrocarbons indicate that shock heating induces breaking of the C-H bonds, and the compression encourages condensation of the dissociated carbon atoms into a residue.¹⁶ If we

assume that the hydrocarbons have been completely converted into a mixture of condensed carbon and molecular hydrogen, we can use known equations of state for each of these materials that have been obtained from shock-wave studies to compute high-density Hugoniots that are in excellent agreement with the experimental hydrocarbon data. The results of similar calculations for molecular methane¹⁵ are also in agreement with the experimental data suggesting that the final product is a mixture of hydrogen and a carbon residue possibly in the diamond or metallic phase.¹⁷ Shockwave data on diamond and graphite shows that the carbon condensate at a few megabars will be denser than NH₃ or H₂O and, unless it is highly soluble in the fluids, may separate out and sink below to form a denser layer.

Shockwave data on water and ammonia, including electrical conductivities, have been measured over part of the Uranus (Neptune) pressure-temperature range. The electrical conductivity data shows that above 0.2 Mbar and about 2000 Kelvin the conductivities become constant at about 20 to 30 mho/cm, as if the processes leading to ionization have become saturated. It would appear that water has become fully ionized. For ammonia similar results have been observed. Consequently we must conclude that in the Uranus and Neptune "ice" layer H₂O and NH₃ are not molecular but ionic, and that the carbon in methane has been converted to a diamond or metallic phase with molecular or metallic hydrogen.

REFERENCES

*Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract #W-7405-Eng-48.

1. Slattery, A. L., Icarus 1977, 32, 58.
2. Hubbard, W. B. and MacFarlane, J. J., J. Geophys. Res. 1980, 85, 225.
3. Mitchell, A. C. and Nellis, W. J., Rev. Sci. Instrum., 1981, 52, 347.
4. Anderson, M. S. and Swenson, C. A., Phys. Rev. B 1974, 10, 5184.
5. Mills, R. L., Liebenberg, D. H., Bronson, J. C., and Schmidt, L. C., J. Chem. Phys. 1977, 66, 3076.

6. Mao, H. K. and Bell, P. M., *Science* 1979, 203, 1004; Mills, R. L., Liebenberg, D. H., Bronson, J. C., and Schmidt, L. C., *Rev. Sci. Instrum.* 1980, 51, 891. Diatschenko, V. and Chu, P., *Science* 1981, 212, 1393.
7. Nellis, W. J. and Mitchell, A. C., *private communication* (1981).
8. Silvera, I. F. and Goldman, V. V., *J. Chem. Phys.* 1978, 69, 4209.
9. Mills, R. L., Liebenberg, D. H., and Bronson, J. C., *Phys. Rev. B* 1980, 21, 5137.
10. Besson, J. M. and Pinceaux, J. P., *Science* 1979, 206, 1073; Mills, R. L., Liebenberg, D. H., Bronson, J. C. and Schmidt, L. C., *Rev. Sci. Instrum.* 1980, 51, 891.
11. Stewart, J. W., *J. Phys. Chem. Solids* 1956, 1, 146; Stewart, J. W., *Phys. Rev.* 1963, 129, 1950.
12. Young, D. A., McMahan, A. K. and Ross, M., "Equation of State and Melting Curve of Helium to Very High Pressure", Lawrence Livermore National Laboratory Report UCRL-85788, Livermore, California (1981).
13. Stevenson, D. J., *J. Phys. F: Metal Phys.* 9, 791 (1979).
14. Mitchell, A. C., Kovel, M. I., Nellis, W. J. and Keeler, R. N., in High Pressure Science and Technology Vol. II (Eds. B. Vodar and P. Marteau) (Pergamon Press, Oxford, 1980) p. 1043 and 1048.
15. Ross, M. and Ree, F. H., *J. Chem. Phys.* 1980, 73, 6146.
16. Ree, F. H., *J. Chem. Phys.* 1979, 70, 974.
17. Ross, M., *Nature* 1981, to be published.