

IMPLICATIONS OF SHOCK WAVE EXPERIMENTS WITH PRECOMPRESSED MATERIALS FOR GIANT PLANET INTERIORS

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Abstract. This work uses density functional molecular dynamics simulations of fluid helium at high pressure to examine how shock wave experiments with precompressed samples can help characterizing the interior of giant planets. In particular, we analyze how large of a precompression is needed to probe a certain depth in a planet's gas envelope. We find that precompressions of up to 0.1, 1.0, 10, or 100 GPa are needed to characterized 2.5, 5.9, 18, to 63% of Jupiter's envelope by mass.

Keywords: shock waves, giant planet interiors, high pressure helium, Hugoniot curves, equation of state

INTRODUCTION

Shock wave experiments have served a the primary experimental technique to study material at high pressure and temperature. Laser shocks [1, 2] as well as magnetically driven shocks [3, 4] enable us to reaches megabar pressures and temperature of tens of thousands of degrees Kelvin. The main advantage of this technique is that it requires one to measure only the velocity of the shock front, u_s , and that of the impactor, u_p , in order to obtain direct information about the equation of state. The conservation of mass, momentum, and energy [5] across the shock front relates the initial (E_1, P_1, V_1) and the final (E_2, P_2, V_2) internal energies, pressures and volumes of the material,

$$P_2 - P_1 = \rho_1 u_s u_p \quad , \quad (1)$$

$$\frac{\rho_2}{\rho_1} = \frac{u_s}{u_s - u_p} \quad , \quad (2)$$

$$(E_2 - E_1) + \frac{1}{2}(P_2 + P_1)(V_2 - V_1) = 0 \quad . \quad (3)$$

It is assumed that the shocked material reaches thermal equilibrium during the experiment that typically last on the order of nanoseconds. This assumption is

well justified in most cases unless the shock triggers a phase transformation, e.g. freezing under shock loading, or a slow chemical reaction that is a bit more complex that the mere dissociation of molecules, which occurs very fast.

One disadvantage of shock experiments is that one cannot control the temperature independently from the shock pressure. The velocity of the impactor, also called particle velocity, and the equation of state of the sample material uniquely determine the final temperature, pressure, and density. The collection of all final states that can be reached for different particle velocities is called a Hugoniot curve (Fig. 1).

Initially the compression ratio increases with the particle velocity but above a certain value, most of the shock energy is converted to heating the sample rather than compressing it. For the main constituents in giant gas planets, hydrogen and helium, the maximum compression ratios, V_1/V_2 , are 4.3 [6] and 5.24 [7] respectively. The compression ratio rarely reaches values that are much than that. The maximum shock compression ratio is controlled by the balance of excitations of internal degrees of freedom, which increase the compression, and interaction ef-

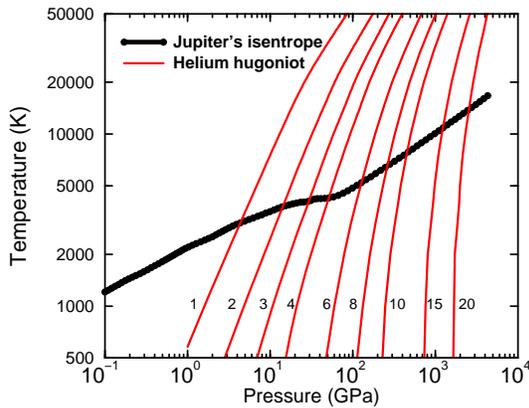


FIGURE 1. Single shock helium Hugoniot curves for different precompression ratios, V_0/V_1 as indicated by the labels, are compared with Jupiter’s isentrope.

fects that reduce the compression [7].

As a result of this limitation for the attainable density, it becomes rather difficult to characterize the interior of planets with shock experiments alone. The shock Hugoniot curves rise much faster in a temperature-pressure diagram than planetary isentropes. Figure 1 illustrates this for helium as a sample material.

This impasse can now be addressed with a new experimental technique [8] that combines static and dynamic compression. By first compressing the sample statically in a diamond anvil cell, the starting density can be sufficiently increased so that a subsequent shock experiment yields equation of state data along a different Hugoniot curve at higher density. Although the compression ratio has been shown to be reduced as a result of the precompression [7], the absolute densities are of course higher due to the precompression. Therefore a larger section of the giant planet interiors can be studied. The purpose of the article is to understand quantitatively how much of a precompression is needed to characterize a substantial part of Jupiter’s gaseous envelope.

METHODS

To characterize the properties of helium at high pressure and temperature, we use density functional molecular dynamics (DFT-MD) computer simula-

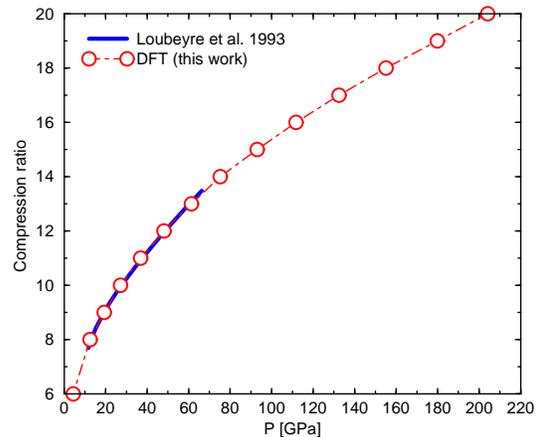


FIGURE 2. Cold curve for solid helium in the h.c.p. phase. The static compression ratio, V_0/V_1 with $V_0 = 32.4$ cm^3/mol , is plotted as function of pressure. The experimental results [13] were obtained with diamond anvil cell measurement and compare favorably with static density functional calculations performed at $T=0$ under hydrostatic conditions.

tion that we perform with the Vienna Ab-initio Simulation Package [9]. The simulation were performed with 64 atoms in the unit cell using Born Oppenheimer molecular dynamics that derive the instantaneous forces from an electronic structure calculation. We used the Perdew-Burke-Ernzerhof generalized gradient approximation [10] for the exchange-correlation energy, and Γ -point sampling of the Brillouin zone. Since electronic excitation are important to characterize helium Hugoniot curve above 10000 K [7], we used a finite temperature Mermin functional to model electronic excitations in thermal equilibrium. More details about the simulation and discussion of finite size corrections can be found in Refs. [7, 11, 12]. We derived the equation of state of dense fluid helium by performing DFT-MD simulations for large grid of density-temperature points and obtained the shock Hugoniot curves by solving Eq. 3.

The static DFT calculations used to derive the cold curve in Fig. 2 were performed with $6 \times 6 \times 6$ k-point mesh in a two atom h.c.p. unit cell under hydrostatic conditions.

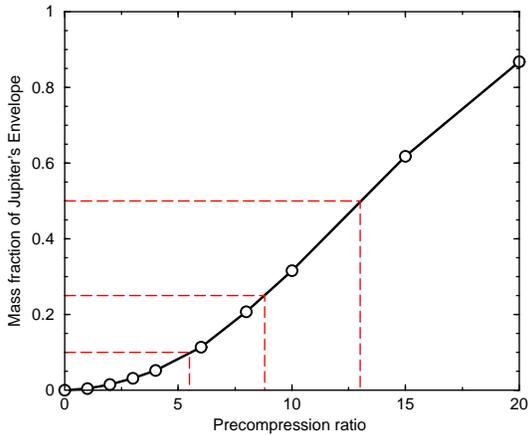


FIGURE 3. Mass fraction of Jupiter’s envelop that can be probed with different precompressions is shown as a function the precompression ratio, $\eta = V_0/V_1$. The dashed lines were included as guide to the eye.

RESULTS

Figure 1 shows a family of shock Hugoniot curves up to a 20-fold precompression. We characterize the precompression in terms of volume change compared to the ambient pressure value of $V_0=32.4$ cm^3/mol [14]. While static diamond anvil cell experiments have explored the pressures beyond 300 GPa [15], there are currently a number of limitations for the precompression pressure in shock experiments. Larger pressures imply thicker diamond windows that require a more powerful shock driver and make it more challenging to launch a planar shock. Reducing the sample size in order to reach a higher precompression makes the diagnostics more difficult.

Let us now assume that we have a particular experimental setup that allows us to launch shocks into a sample that has been precompressed up a maximum initial pressure P_1^* . This translates into a maximum precompression ratio, η^* , that can be inferred from the cold curve [13, 16, 17] shown in Fig. 2 where we compared our static DFT calculation with experimental results. In Fig. 1, we find the pressure, P_2^* , where this particular Hugoniot curve intersects with Jupiter’s isentrope, and can therefore infer the maximum depth in Jupiter’s envelope that we can probe with this particular experimental setup. Since it should always be easier to repeat the experiment

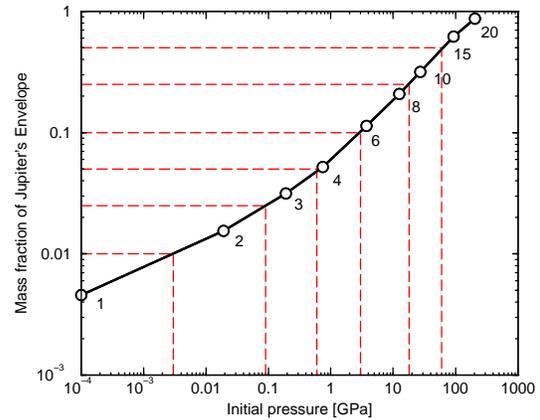


FIGURE 4. Mass fraction of Jupiter’s envelop that can be probed with different precompressions is shown as a function of the initial pressure. The dashed lines were included as guide to the eye. The labels give the precompression ratio, V_0/V_1 , for each circle.

for smaller precompression, we can map out Jupiter’s isentrope for all $P_2 < P_2^*$.

One can now ask the question how deep into Jupiter’s interior one is able to probe. However, Jupiter is an oblate object due to its rapid rotation, and P_2^* cannot be mapped directly into a radius without approximating the planet by a sphere. It is therefore more appropriate to ask what mass fraction of the total gas in the envelop is at pressures less than P_2^* . This way one can map a maximum initial pressure P_1^* into a mass fraction of the planet that can be probed experimentally. Discussing this in terms of the a mass fraction, rather than in terms of depth, is particularly meaningful because giant planet interior models are most sensitive to the equation of state where most of the planet’s mass is. For Jupiter, this is where hydrogen is metallic and consequently a large number experimental and theoretical studies have been devoted to hydrogen under such extreme conditions.

Figures 3 and 4 show the mass fraction as function of precompression ratio and as function of initial pressure, P_1^* . It becomes clear that a substantial precompression pressure is needed to study Jupiter. With precompressions of up to 0.1, 1.0, 10, or 100 GPa are needed to characterized 2.5, 5.9, 18, to 63% of Jupiter’s envelop by mass. While a precompression up 1 GPa increase the sample density approxi-

mately 5-fold, it is not sufficient to characterize more than 5.9% of Jupiter's mass. Since precompression above 1 GPa cannot readily be obtained yet, one might consider performing double or triple shock experiments [18] with precompressed samples.

CONCLUSIONS

We performed density functional molecular dynamics simulations to characterize the fluid helium at high pressure and temperature. We derived the shock Hugoniot curve up to precompression ratio of 20. By comparing the Hugoniot curve with Jupiter's isentrope, we conclude that precompressions of up one megabar would be needed to characterize a substantial fraction of Jupiter's envelop. Such large precompression could be difficult to obtain due to limitations of shock drive and a minimum sample size that is required. As a conclusion, we suggest that venue of precompressed shock experiments with two or more reverberating shocks should be explored.

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