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2006 J. Phys. A: Math. Gen. 39 4479

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Equation of state for dense hydrogen and helium: application to astrophysics

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Received 17 September 2005, in final form 4 January 2006

Published 7 April 2006

Online at stacks.iop.org/JPhysA/39/4479

Abstract

We present theoretical results for the equation of state of hydrogen and helium applying the chemical picture which treats the elementary charged particles (electrons, ions) and neutral bound states (atoms, molecules) on an equal footing. The chemical equilibrium for dissociation and ionization processes is solved accounting for nonideality corrections. We compare our results with experiments and other theoretical models and calculate pressures and temperatures in jupiter's interior.

PACS numbers: 51.30+i, 52.25.Jm, 52.25.Kn, 96.35.Mz

1. Introduction

The properties of hydrogen (or deuterium), helium and their mixtures at high pressure are of great interest for models of the interiors of stars and giant planets as well as for inertial confinement fusion experiments. Thus, precise knowledge of the equation of state (EOS) of hydrogen and helium is needed for a large domain of densities and temperatures, especially for high densities as typical for condensed matter and temperatures of several eV, i.e. for *warm dense matter*.

We present results for the EOS of dense hydrogen and helium and their mixtures based on the chemical picture which treats pressure dissociation and ionization processes via laws of mass action, see [1–5] for details. Shock-wave experiments [6–12] were performed to probe the EOS in the high-pressure region. Furthermore, a transition from nonmetallic to metallic behaviour is derived from the strong increase of the electrical conductivity [13, 14] and reflectivity [15] above 40 GPa. Some theoretical models predict that this electronic transition is accompanied by a thermodynamic phase instability, the *plasma phase transition* (PPT) [16–19], which would affect models of planetary interiors and the evolution of giant planets [20–22].

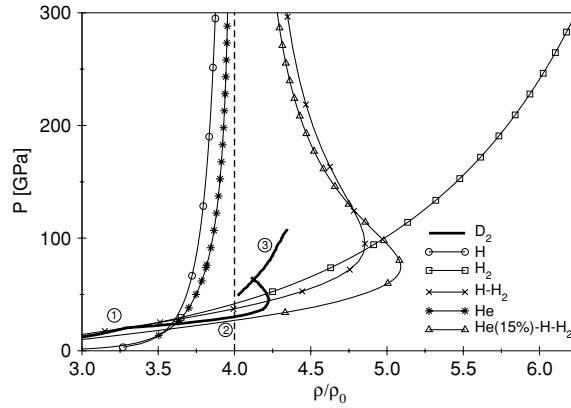


Figure 1. Hugoniot curves as a function of the compression ratio for hydrogen (atomic, molecular, H–H₂ mixture with dissociation), atomic helium and a hydrogen–helium mixture (15% He mass fraction) using the EOS from FVT. We compare with fits to a series of new experimental data for deuterium in three pressure regions 1–3 [12].

2. Equation of state within the chemical picture

In the chemical picture, hydrogen and helium are considered as a mixture of a plasma component (electrons and ions) and a neutral component (atoms and molecules). Pressure dissociation ($\text{H}_2 \rightleftharpoons 2\text{H}$) and ionization processes (e.g. $\text{H} \rightleftharpoons \text{e} + \text{p}$) are taken into account via respective laws of mass action so that a transition from a molecular or atomic fluid at low temperatures and pressures to a fully ionized, hot plasma above several 10^4 K is described [3, 4]. The EOS calculations start from a linear-mixing expression for the free energy of the neutral (F_0) and charged components (F_{\pm}):

$$F(V, T, \{N\}) = F_0 + F_{\pm} + F_{\text{pol}}. \quad (1)$$

The first two terms contain ideal and interaction parts via $F_0 = F_0^{\text{id}} + F_0^{\text{int}}$ and $F_{\pm} = F_{\pm}^{\text{id}} + F_{\pm}^{\text{int}}$. The third term describes the interaction between charged and neutral particles via a polarization potential [23]. The particle numbers considered here are $\{N\} = \{N_{\text{e}}, N_{\text{p}}, N_{\text{H}}, N_{\text{H}_2}\}$ for hydrogen and $\{N\} = \{N_{\text{e}}, N_{\text{He}^{2+}}, N_{\text{He}^+}, N_{\text{He}}\}$ for helium, respectively. Other quantities such as pressure P , chemical potential μ or internal energy U follow from equation (1) via standard thermodynamic relations.

The excess contribution F_0^{int} is determined within fluid variational theory (FVT). Starting from a reference system of hard spheres, effective potentials of the exponential-6-type are used for the interaction between the neutral particles, see [3]. Pressure dissociation in hydrogen is treated self-consistently via the chemical equilibrium condition $\mu_{\text{H}_2} = 2\mu_{\text{H}}$ [24, 25]. Thermodynamic properties are derived from the minimum of F with respect to the hard sphere diameters and the dissociation degree.

We show Hugoniot curves as a function of the compression ratio derived from FVT for hypothetical pure atomic (H) and molecular hydrogen fluids (H₂), the H–H₂ mixture with self-consistent treatment of dissociation, atomic helium (He) and a hydrogen–helium mixture in figure 1. We have used in all cases an initial density of $\varrho_0 = 0.0855 \text{ g cm}^{-3}$ in order to allow for a direct comparison with experiments for deuterium which are performed with just the double initial density, i.e. $\varrho_0(\text{D}_2) = 0.171 \text{ g cm}^{-3}$. The factor 2 between the initial masses of D₂

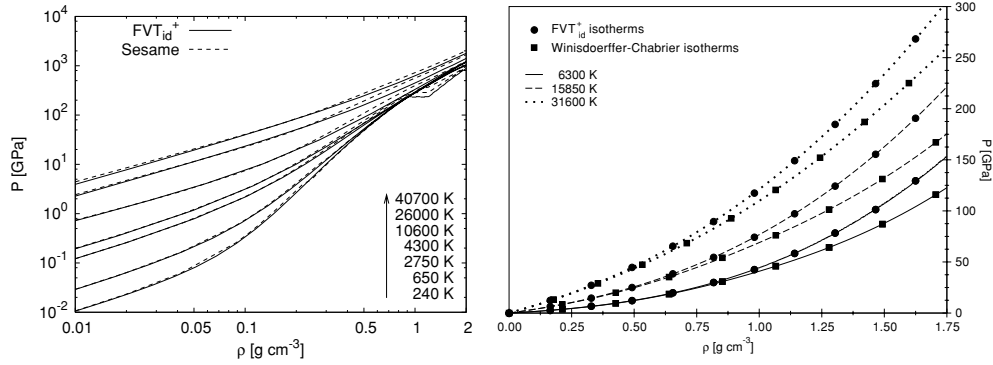


Figure 2. EOS for hydrogen (left) and helium (right) by using the FVT_{id}^+ model. The hydrogen EOS is compared with the Sesame tables [30], and the helium EOS with a similar chemical model of Winisoerffer and Chabrier [34].

and H_2 is exactly cancelled by the specific internal energy term in the Hugoniot relation. Note that the initial density of hydrogen used in shock-wave experiments is $\rho_0 = 0.071 \text{ g cm}^{-3}$ so that the measured Hugoniot curves for hydrogen and deuterium are not the same, see [26]. In this way, we can compare our $H-H_2$ curve with accurate fits to new data for deuterium obtained in a series of shock-wave experiments [12]. The fits were constructed for three different pressure regions 1–3; the agreement is good up to about 40 GPa. For higher pressures (region 3), FVT yields a higher compression than the experiments. A more detailed comparison of FVT results with shock-wave experiments is given in [3–5].

The Hugoniot curves for the pure atomic systems approach four-fold compression at ultra-high pressures, whereas the pure molecular system without dissociation tends to eight-fold compression because of the internal degrees of freedom of the molecules (rotation and vibration). Self-consistent treatment of pressure dissociation for the $H-H_2$ system via the relation $\mu_{H_2} = 2\mu_H$ yields a maximum compression of about 4.75, see [25]. The FVT results also agree well with reaction ensemble Monte Carlo simulations [27, 28]. Double-shock experiments performed with the Omega laser in deuterium support such a behaviour [29], while reverberation measurements with the Z accelerator [9] are in accordance with a stiffer EOS such as Sesame [30] or PIMC simulations [31] which give a maximum compression of about 4.5. The new experiments [12] displayed in figure 1 support strongly such a stiffer behaviour of the hydrogen (deuterium) EOS. The hydrogen–helium mixture shows almost the same behaviour as the $H-H_2$ system but a slightly increased compressibility due to the helium fraction.

In a next step, we consider the plasma contribution F_{\pm} in equation (1) in order to treat the influence of ionization processes on the high-pressure EOS. The excess contribution F_{\pm}^{int} has been included in earlier work devoted to the stability behaviour of the EOS and the PPT by using Padé approximations [32, 33]. For simplicity, we neglect this contribution here and label the corresponding model as FVT_{id}^+ , see [3, 4] for details. We show the resulting pressure isotherms as a function of the density for hydrogen and helium in figure 2. The agreement with the respective comparative data is very good for both elements up to 0.5 g cm^{-3} . For higher densities, the FVT_{id}^+ model gives systematically lower pressures for hydrogen and, contrary, higher pressures for helium. The Sesame data show a phase instability for the lowest temperatures at about 1 g cm^{-3} which is treated by a Maxwell construction.

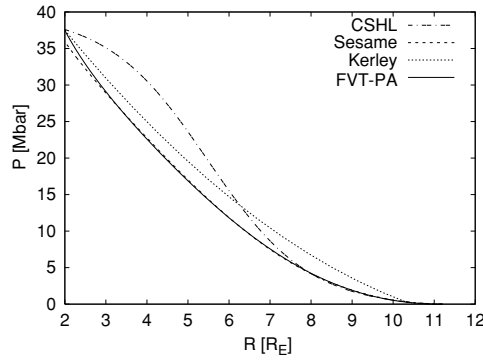


Figure 3. Pressure profile along the radius of Jupiter measured in the earth radii R_E , see also [4]. The FVT-PA result is compared with the Sesame tables [30], Kerley’s revised EOS [37] and a three-shell model of Chabrier *et al* (CSHL) [21].

3. Planetary interiors

The application of the different EOS for hydrogen and helium in models for giant planets and the comparison of their predicted internal structure with observational parameters is an alternative test besides high-pressure experiments, see [35–37]. Giant planets such as Jupiter consist mainly of hydrogen and helium, forming a cold molecular fluid in the outer envelope and a pressure ionized plasma in the deeper interior as indicated by the existence of a magnetic field. Assuming a simple, two-layer model (solid core and homogeneous fluid above), the observational parameters to be fitted are the total mass M of the planet, its equatorial radius R_{eq} up to the 1 bar level, the lowest gravitational moment J_2 and the temperature T at the outer boundary; for more realistic multilayer planetary models, see [35, 36, 38]. The interior profile is then calculated by integration of the equation of hydrostatic equilibrium

$$\frac{1}{\varrho(r, \theta)} \frac{dP(r, \theta)}{dr(\theta)} = \frac{d}{dr(\theta)} \{V(r, \theta) + Q(r, \theta)\} \quad (2)$$

along the isentrope defined by the outer boundary; $V(r, \theta)$ is the gravitational and $Q(r, \theta)$ is the centrifugal potential. The dependence on the polar angle θ accounts for shape deformations due to rotation. The gravitational potential is expanded into a series of Legendre polynomials $P_{2i}(\cos \theta)$ with the gravitational moments J_{2i} as expansion coefficients [35]. J_{2i} are sensitive to the mass distribution and, thus, can serve as measures of the quality of the EOS used. We apply the *theory of figures* [39] to solve the equation of hydrostatic equilibrium (2) including rotation. For densities less than 1 g cm^{-3} we use the EOS from the FVT_{id}⁺ model. For higher densities as relevant for Jupiter’s deeper interior (but not reached in current shock-wave experiments), we take into account also the excess contributions F_{\pm}^{int} of the plasma component in equation (1) via Padé approximations [40] and denote this slightly modified model by FVT-PA.

With the given equations of state for pure hydrogen and helium, we calculate the thermodynamic properties of a H–He mixture via the additive volume rule. It states that extensive variables such as the internal energy and the entropy are strictly added. In accordance with [21] we neglect the entropy of mixing.

The calculated pressure profile (temperature profiles are given in [4]) along the radius of Jupiter agrees almost perfectly with the predictions of the original Sesame EOS [30], see figure 3. Kerley’s revised Sesame EOS [37] and a three-shell model of Chabrier *et al* (CSHL)

[21] give systematically higher pressures, also due to the consideration of heavier elements than helium. The helium fraction Y is used in our calculation to reproduce the gravitational moment J_2 . The result of the FVT-PA model is 27%—which is just the helium abundance in the protosolar cloud. This value defines a genuine lower bound for Y because heavier elements have to be considered as well. Their fraction Z is given by the difference between the calculated helium fraction Y and 27%. Therefore, no fraction of heavier elements could be added in our present FVT-PA model, which indicates that this hydrogen EOS is probably too soft and that the maximum compression along the Hugoniot curve should be below 5.5.

4. Conclusions

In this paper, we have applied a chemical model to calculate the EOS of hydrogen and helium and the pressure profile in jupiter. Details of the thermodynamic properties such as the maximum compression along the Hugoniot curve, the influence of nonideality corrections on the combined dissociation–ionization equilibrium in hydrogen–helium mixtures, or the stability behaviour of the EOS are the subject of further work. A generalization of the present two-layer model to a multilayer model is intended to get a more realistic description of planetary interiors.

Acknowledgments

We thank B Militzer, W-D Kraeft, W J Nellis and W Ebeling for helpful comments. This work was supported by the Deutsche Forschungsgemeinschaft within the SFB 652.

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