

Equation of state of dense hydrogen and phase transitions

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The equation of state (EOS) of warm dense hydrogen is treated theoretically by a free energy approach. At low densities hydrogen is a molecular fluid which can be described by fluid variational theory. Dissociation of molecules is treated self-consistently and thermodynamic properties of the neutral fluid can be given via standard relations, see [1] for details.

At high densities hydrogen is predicted to be in a metallic-like state. In the chemical picture the fluid and plasma states are mixed and the total free energy is minimal in chemical equilibrium. Therefore, the chemical potentials of the molecular system, of the atoms, and of the electrons and ions are equal and a coupled system of mass action laws is derived which gives the composition of partially ionized hydrogen plasma. In simplified calculations applied to hydrogen and deuterium the charged particles were treated as ideal plasma. The partition function of the atoms was supposed to be density-dependent using an expression of Kerley [2] which leads to full ionization at high densities. Comparison of Hugoniot curves with shock wave experiments and other theories is performed in Fig. 1.

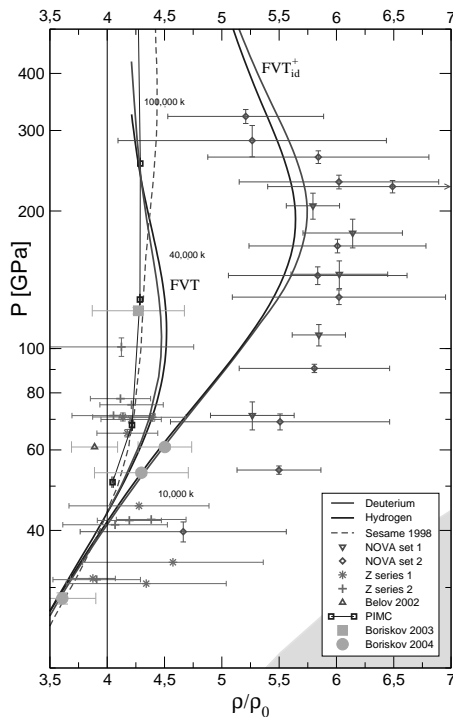


Figure 1: Theoretical and experimental Hugoniot curves as function of the compression ratio ρ/ρ_0 . ρ_0 is 0.085 g/cm^3 and 0.17 g/cm^3 for hydrogen and deuterium, respectively. Further explanation is given in [1].

In extended calculations including the correlations of charged particles by use of Padé approximations [3] the occurrence of a plasma phase transition (PPT) is observed. These calculations show a rapid increase of ionization at a density of about 1 g/cm^3 . This increase leads to a thermodynamic instability which is interpreted as a first-order phase transition. To reach full ionization at even higher densities an excluded volume concept is considered in the ideal parts of the thermodynamic functions.

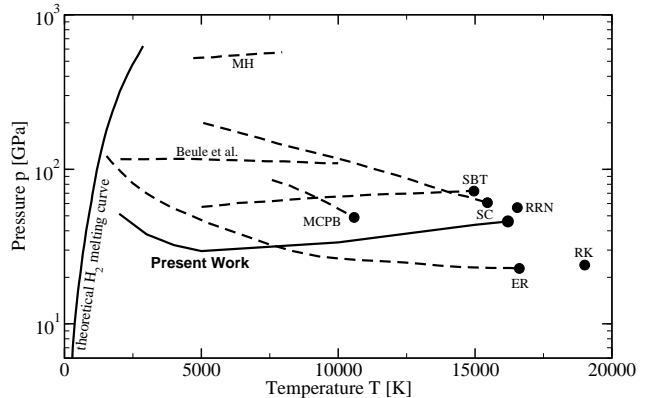


Figure 2: Phase diagram of hydrogen: Coexistence lines and critical points of the PPT arising from the present work (solid line) compared with previous calculations (dashed lines): RRN[4], SC[5], ER[6], SBT[7], RK[8], MCPB[9], MH[10], Beule et al.[11]. The theoretical H_2 melting curve is from [12].

The coexistence curve of hydrogen shown in Fig. 2 is in agreement with the predictions of other theories. The critical point is at about 16000 K and a pressure of 0.5 Mbar. The pressure is slightly decreasing with lowering the temperature and rises again for temperatures lower than 5000 K. The coexistence curve approaches the theoretical H_2 melting line in the pressure region around 0.5 Mbar.

It is planned to use this EOS as input for modeling the interiors of Giant Planets like Jupiter and Saturn which consist mainly of hydrogen and helium. Further possible applications are hydrodynamic calculations for heavy ion heated targets.

References

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