Equation of state for hot dense matter using a relativistic screened hydrogenic model

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Introduction

The study of matter under conditions of high density, pressure, and temperature is a valuable subject for inertial confinement fusion (ICF), astrophysical phenomena, high-power laser interaction with matter, etc. In all these cases, matter is heated and compressed by strong shocks to high pressures and temperatures, becomes partially or completely ionized via thermal or pressure ionization, and is in the form of a dense plasma. The thermodynamics and the hydrodynamics of hot dense plasmas cannot be predicted without the knowledge of the equation of state (EOS) that describes how a material reacts to pressure and how much energy is involved. Therefore, the equation of state often takes the form of pressure and energy as functions of density and temperature. Furthermore, EOS data must be obtained in a timely manner in order to be useful as input in hydrodynamic codes. By this reason, the use of fast, robust and reasonably accurate atomic models, is necessary for computing the EOS of a material.

We use the ATMED code [1] to compute the equation of state of hot dense plasmas under LTE conditions in the average atom framework, using a Screened Hydrogenic Model based on a new set of screened constants including the relativistic splitting of the energy levels [2]. To validate the code, we have carried out the computation of the Rankine-Hugoniot curve for plasmas of elements with medium and high Z values.

Description of the model

The model adopts the assumption that ionic and electron quantities are additive to sufficient accuracy so the Helmholtz free energy per unit of mass can be written in the form:

$$F(\rho, T) = F_i(\rho, T) + F_e(\rho, T) - F_e(\rho, T_c) + F_c(\rho) \tag{1}$$

In this equation ρ is the plasma density, T is the plasma temperature, $F_i(\rho, T)$ is the ion free energy, $F_e(\rho, T)$ is the electron free energy calculated from the spherical-cell Thomas-Fermi theory and $F_c(\rho)$ is the energy of the material at zero temperature T_c. The ion contribution to the energy is obtained from the Cowan ion equation of state, a single analytic model which

combines general laws in several limiting cases, such as the ideal gas law, the fluid scaling law, the Lindermann melting law or the Gruneisen pressure law. This model is divided into two parts, a structural part which gives the thermodynamic functions: pressure p_i, internal energy E_i, entropy S_i, and Helmholtz free energy F_i, and an empirical part which predicts the melting temperature $T_m(\rho)$ and the Debye temperature $\Theta_D(\rho)$ [3].

The electronic Helmholtz free energy per unit of mass of the plasma is [4]:

$$F_e(\rho,T) = F_{bound}(\rho,T) + F_{free}(\rho,T) + F_{ion-sphere}(\rho,T) \tag{2}$$

where $F_{bound} = E_{bound} - T \cdot S_{bound}$ is the free energy of the bound electrons in the average atom, F_{free} is the energy of a homogeneous free electron gas, and $F_{ion-sphere}$ is introduced to account for the effect of plasma environment on the bound electronic energy levels, i.e. the continuum lowering. The internal energy $E_{bound} = \sum_k P_k \cdot \varepsilon_k$ is the energy of an electronic configuration $\{P_k\}$, where ε_k represents the Dirac's eigenvalue which is calculated using a new relativistic hydrogenic model [2]. S_{bound} is the entropy associated with the electronic configuration of the average atom model:

$$S_{shm} = -k_B \sum_k \left[P_k \log\left(\frac{P_k}{D_k}\right) + (D_k - P_k)\log\left(\frac{D_k - P_k}{D_k}\right) \right] \tag{3}$$

being D_k the fractional electronic degeneracy of the subshell k including dense plasma effects [4]. The electronic free energy is given by the equation:

$$F_{free}(\rho,T_e) = -\bar{Z}k_B T \left[\eta_e - \frac{2}{3}\frac{f_{\frac{3}{2}}(\eta_e)}{f_{\frac{1}{2}}(\eta_e)} \right], \qquad \bar{Z} = \frac{4}{\sqrt{\pi}}\frac{A}{\rho N_A}\left(\frac{m_e k_B T_e}{2\pi\hbar^2}\right)^{\frac{3}{2}} f_{1/2}(\eta_e) \tag{4}$$

where $\bar{Z}$ is the average ionization of the plasma, k_B is the Boltzmann constant, η_e is the electron reduced chemical potential and $f_\alpha(\eta_e)$ is the Fermi-Dirac integral of order α. The ion-sphere energy is:

$$F_{ion-sphere} = -\frac{9}{10}\frac{\bar{Z}^2 e^2}{R_0} = -\frac{1}{2}\bar{Z}\Delta I \tag{5}$$

and

$$\Delta I = \frac{9}{5}\frac{\bar{Z}e^2}{R_0}, \qquad R_0 = \left(\frac{4\pi}{3}\frac{\rho N_A}{A}\right)^{-1/3} \tag{6}$$

are the ionization potential lowering and the ion-sphere radius, respectively. In these equations e is the electron charge, N_A is the Avogadro number and A is the molar mass.

Since the contribution $F_e(\rho,T)$ calculated from the Thomas-Fermi model is not valid for $T \to 0$ then $F_e(\rho,0)$ must be substracted from electron free energy, and replaced by $F_c(\rho)$, which constitutes the cold curve. In our model, the zero temperature isotherm is obtained from
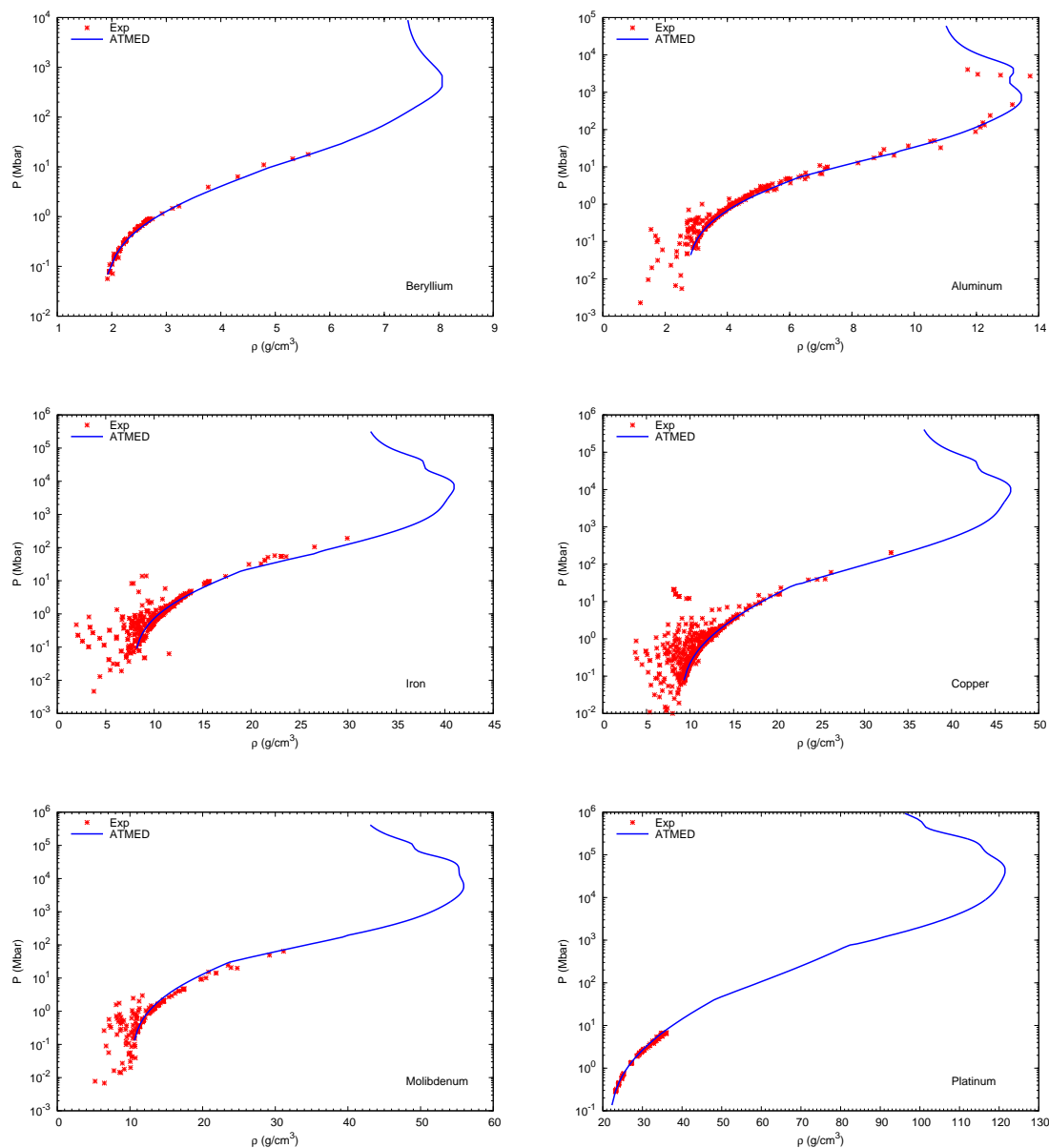
Figure 1: Principal Hugoniot curves calculated using ATMED code for several elements are compared with experimental data. Initial conditions are $\rho_0 = \rho_s$ and $T = 300$ K.

the scaled binding energy formula for solids [5]. Total pressure p, entropy S and internal energy E are derived from Helmholtz free energy $F(\rho, T)$ according to the equations:

$$p = \rho^2 \frac{\partial F}{\partial \rho}, \qquad S = -\frac{\partial F}{\partial T}, \qquad E = F + T \cdot S \tag{7}$$

Results

The correct reproduction of the Rankine-Hugoniot curves or shock adiabats constitutes the best way to validate a model of equation of state. The Hugoniot curves are obtained from the
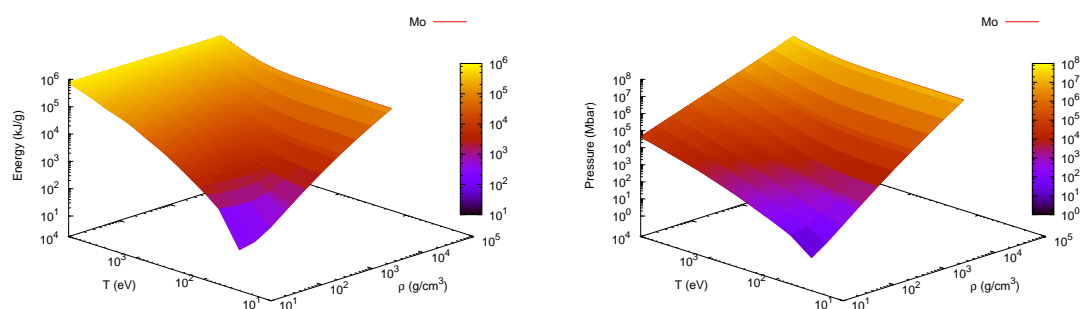
Figure 2: Energy and pressure surfaces for molybdenum computed with ATMED.

equation:

$$E - E_0 = \frac{1}{2}(p - p_0)(\frac{1}{\rho_0} - \frac{1}{\rho})$$ (8)

which represents the energy conservation law for a shock wave, and where subscript 0 characterizes the initial state. Main Hugoniot curves have $p_0 = 0$, $\rho_0 = \rho_s$ and $T = 300$ K, being ρ_s the normal solid density. Figure 1 shows principal Hugoniot curves computed with ATMED code for beryllium, aluminum, iron, copper, molybdenum and platinum. As it can be seen results are in good agreement with experimental data obtained from reference [6].

Acknowledgments

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