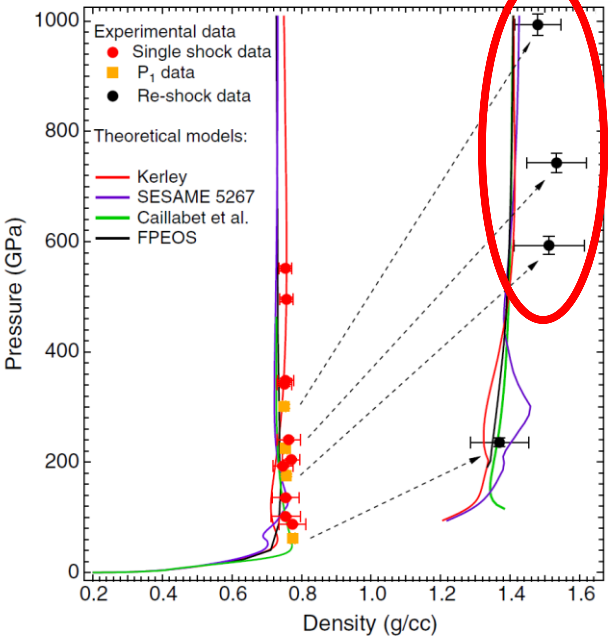
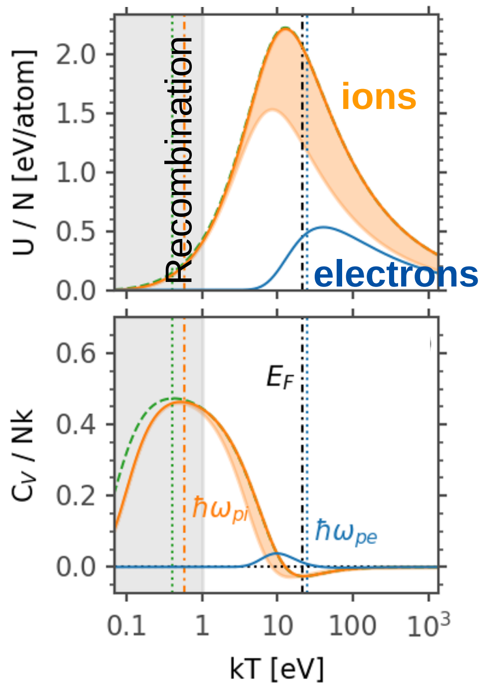
Plasma Waves and the Compressibility of Warm Dense Hydrogen

Fernandez-Pañella (2019)
deuterium re-shock



~1 eV/atom
energy difference

Internal energy of plasma waves



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Division of Plasma Physics
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The heat capacity of plasma waves can explain the high experimental D_2 compressibility near 500 GPa

- Recent shock, re-shock, and sound speed experiments[1,2] report higher compression of deuterium (^2H) near 500 GPa than predicted by models.

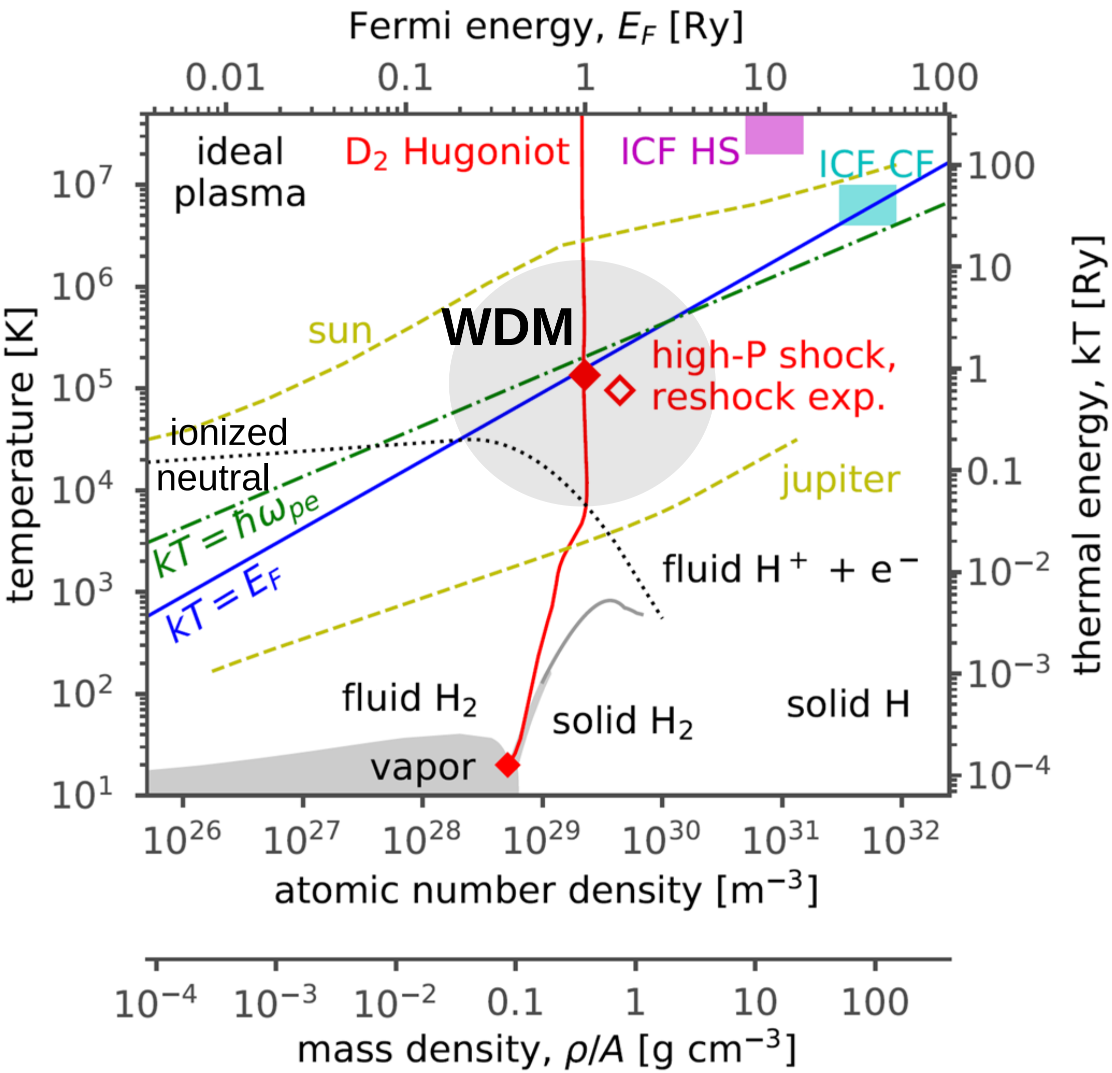
- Using a Debye-type model, a specific heat contribution up to $k_B/2$ per atom is calculated for plasmons in warm dense hydrogen.

- Warm dense matter: the thermal energy, Fermi energy, electron plasmon energy, Coulomb coupling energy, and ionization energy are all approximately and simultaneously equal to 1 Ry (1 Ry = 13.6 eV).

- This specific heat contribution is not explicitly considered in current hydrogen equation of state models, including those of both the “chemical free energy” and “quantum ab initio” varieties.

1. A. Fernandez-Pañella et al, Phys. Rev. Lett. 122, 255702 (2019).
2. D. E. Fratanduono et al, Phys. Plasmas 26, 012710 (2019).

In warm dense matter (WDM), all energies are ~1 Ry



Atomic Energy (Rydberg):

$$E_R = 13.6\ \text{eV}$$

Thermal Energy:

$$E_T = k_B T$$

Fermi Energy:

$$E_F = \left(3\pi^2\right)^{2/3} \frac{\hbar^2}{2m_e} n_e^{2/3}$$

Coulomb Potential Energy:

$$E_C = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{4}{3}\pi n_e\right)^{1/3}$$

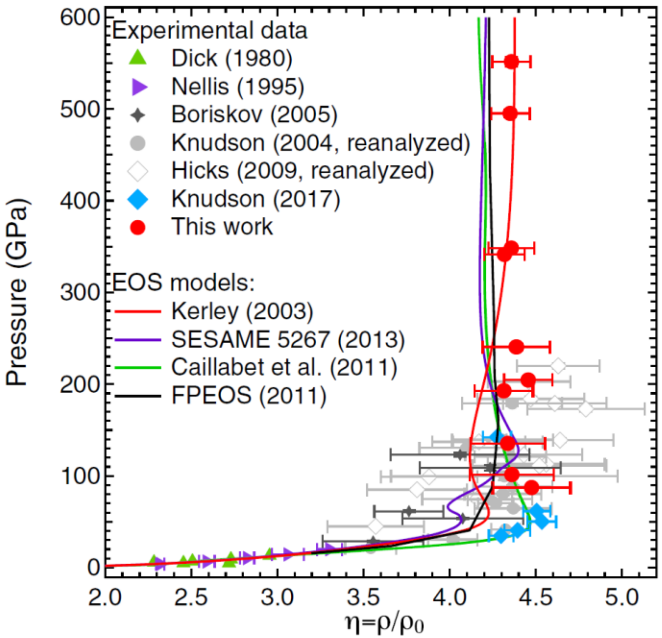
Plasmon Energy:

$$\hbar\omega_{pe} = \hbar\left(\frac{n_e e^2}{\varepsilon_0 m_e}\right)^{1/2}$$

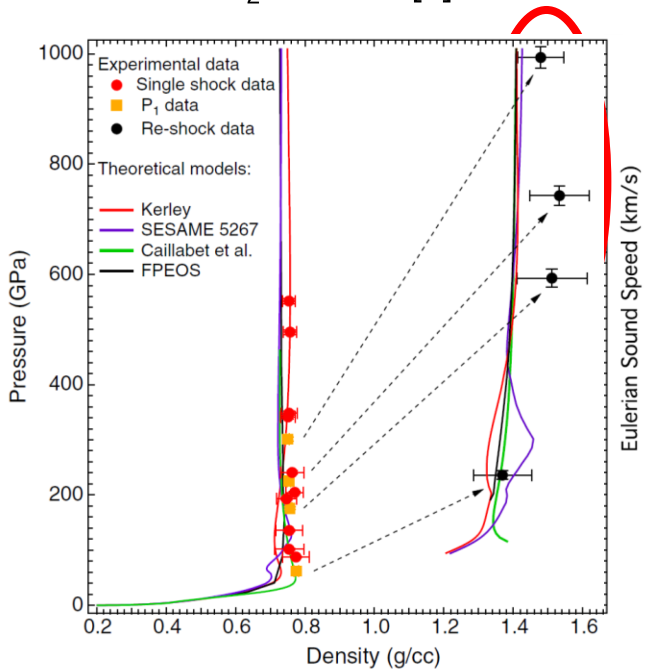
* Contours assume full ionization

Recent experimental data suggest model discrepancies in the high-pressure, high-density D_2 EOS

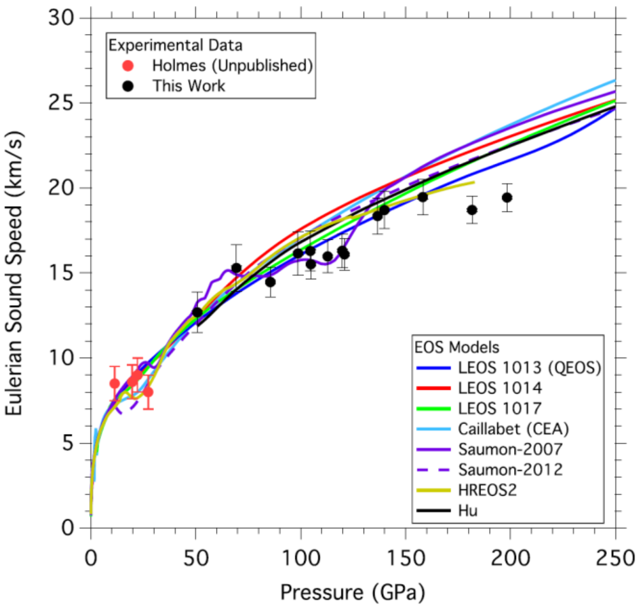
D_2 shock [1]



D_2 reshock [1]



D_2 shock sound speed [2]



This is not a single datum with a 1-sigma discrepancy. This is a systematic discrepancy consistent across 3 different experimental techniques: (1) shock, (2) reshock, (3) sound speed. Each technique has different systematic uncertainties.

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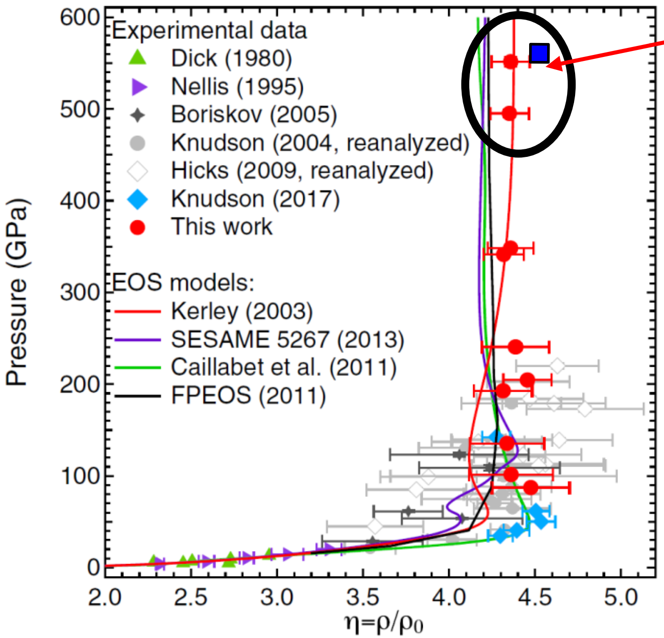
The compression difference can be explained by an additional internal energy of about 1 eV/atom

D_2 shock [1]



~5% (or 8%*) difference in the shock compression.

From Rankine-Hugoniot energy relation:

$$E_1 - E_0 = \frac{1}{2}(P_1 + P_0)\left(\frac{1}{\rho_0} - \frac{1}{\rho_1}\right)$$

Rearrange terms (and define E_0=0):

$$E_1 = \frac{P_1 + P_0}{2\rho_0}\left(1 - \frac{\rho_0}{\rho_1}\right)$$

The different final densities between theory and experiment gives a difference of order **1 eV/atom** in the final internal energy

Let's see if collective plasma oscillations can plausibly account for this energy missing from the models.

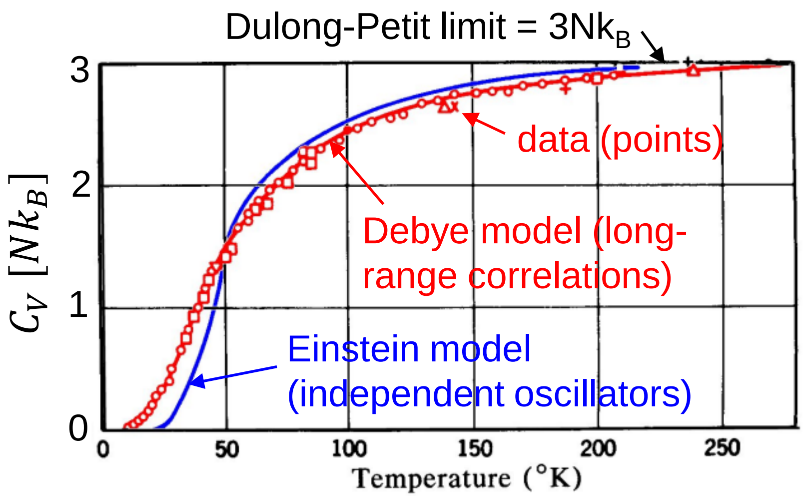
* 8% based on re-analysis using new measurements[1] of shock standard

1. M. C. Marshall et al, Phys. Rev. B 99, 174101 (2019).

Review: heat capacity and the Debye[1] phonon model

- In classical solids at high temperature, heat capacity is $3Nk_B$ for N particles (Dulong-Petit limit)
- At low temperatures, the heat capacity drops as oscillations are "frozen out"
- The Debye model[1] considers long-range correlations in the lattice and is a good representation for most solids.
- For hot plasmas, long-range correlations are usually neglected, since the plasma screening length suppresses its importance.
- However, for warm dense plasmas (moderate coupling) these long-range correlations may again play a role.

Phonon heat capacity in silver



1. P. Debye, Ann. D. Physik 39, 789 (1912).

Debye model[1] for phonon internal energy and C_V

The Debye model for phonon internal energy is:

$$E = \int_0^{q_c} \epsilon(q) g(q) n_{BE}(q)\, dq$$

$\epsilon(q) = \hbar\omega(q)$: dispersion relation
$g(q)$: density of states
$n_{BE}(q)$: occupancy from Bose-Einstein distribution
q_c: cutoff wavenumber (highest supported wavenumber)
c_s: sound speed

Dispersion relation

$$\epsilon(q) = \hbar\omega(q) = \hbar c_s q$$

Density of states

$$g(q) = \frac{Vq^2}{2\pi^2}$$

Bose-Einstein distribution function (zero chemical potential for phonons)

$$n_{BE}(q) = \frac{1}{e^{\hbar c_s q / k_B T} - 1}$$

Cutoff wavenumber is related to the Debye temperature (to reproduce Dulong-Petit limit)

$$q_c = \left(6\pi^2 n\right)^{1/3} = \frac{k_B T_D}{\hbar c_s}$$

Putting it all together, we have expressions for energy and heat capacity

$$E = \frac{V}{2\pi^2} \int_0^{q_c} \frac{\hbar c_s q^3 dq}{e^{\hbar c_s q / k_B T} - 1} \qquad C_V = \left(\frac{\partial E}{\partial T}\right)_V$$

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We can use the Debye model for plasma oscillations

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Dispersion relation

$$\epsilon(q) = \hbar\omega(q)$$

Need to modify the dispersion relation for plasma oscillations[1,2]

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Bose-Einstein distribution function (zero chemical potential for phonons)

$$n_{BE}(q) = \frac{1}{e^{\hbar c_s q/k_B T} - 1}$$

Cutoff wavenumber

$$q_c \propto \frac{1}{\lambda_{screen}}$$

Need to modify the cutoff wavenumber for screening[1,2]

Putting it all together, we have expressions for energy and heat capacity

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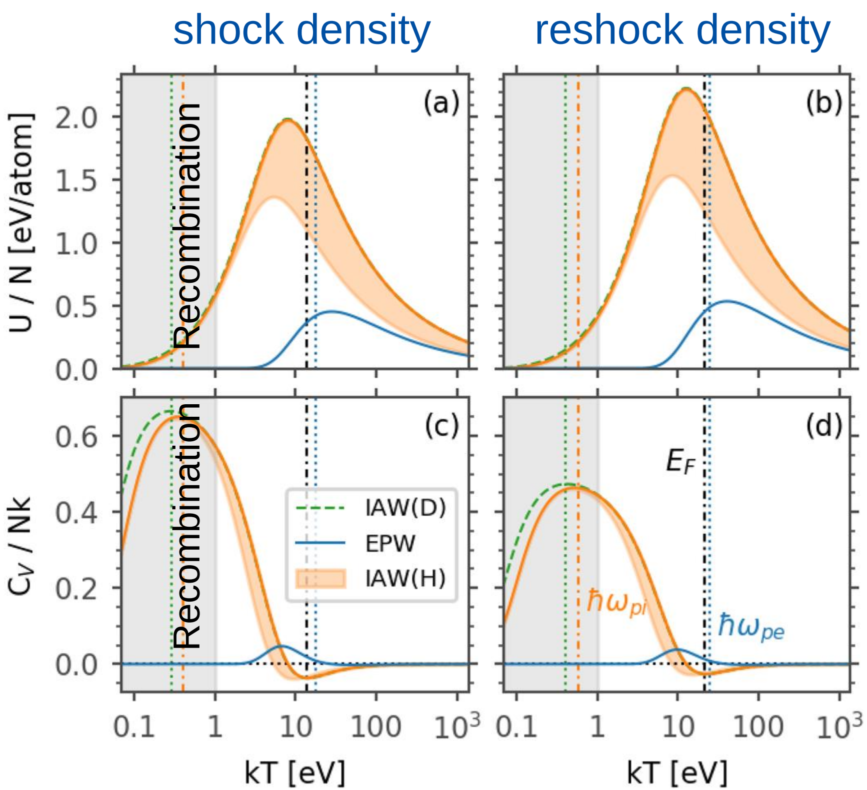
Plasma dispersion and screening for arbitrary degeneracy, eg:

1. Pines and Schrieffer, Phys. Rev. (1962)
2. Melrose and Mushtaq, Phys. Rev. E (2010)

Ion plasma excitations contain sufficient energy to explain the shock compression difference

Energy and heat capacity of plasma oscillations



- Ion acoustic waves may have the ~1eV/atom internal energy required to explain the shock compression discrepancy
- Electron plasma waves have less energy content due to higher frequency and lower Bose-Einstein occupancy factor
- The energy content peaks at a temperature near the Fermi energy, above which plasma screening limits the available oscillation modes

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