Semi-empirical multiphase equation of state of liquid hydrogen.

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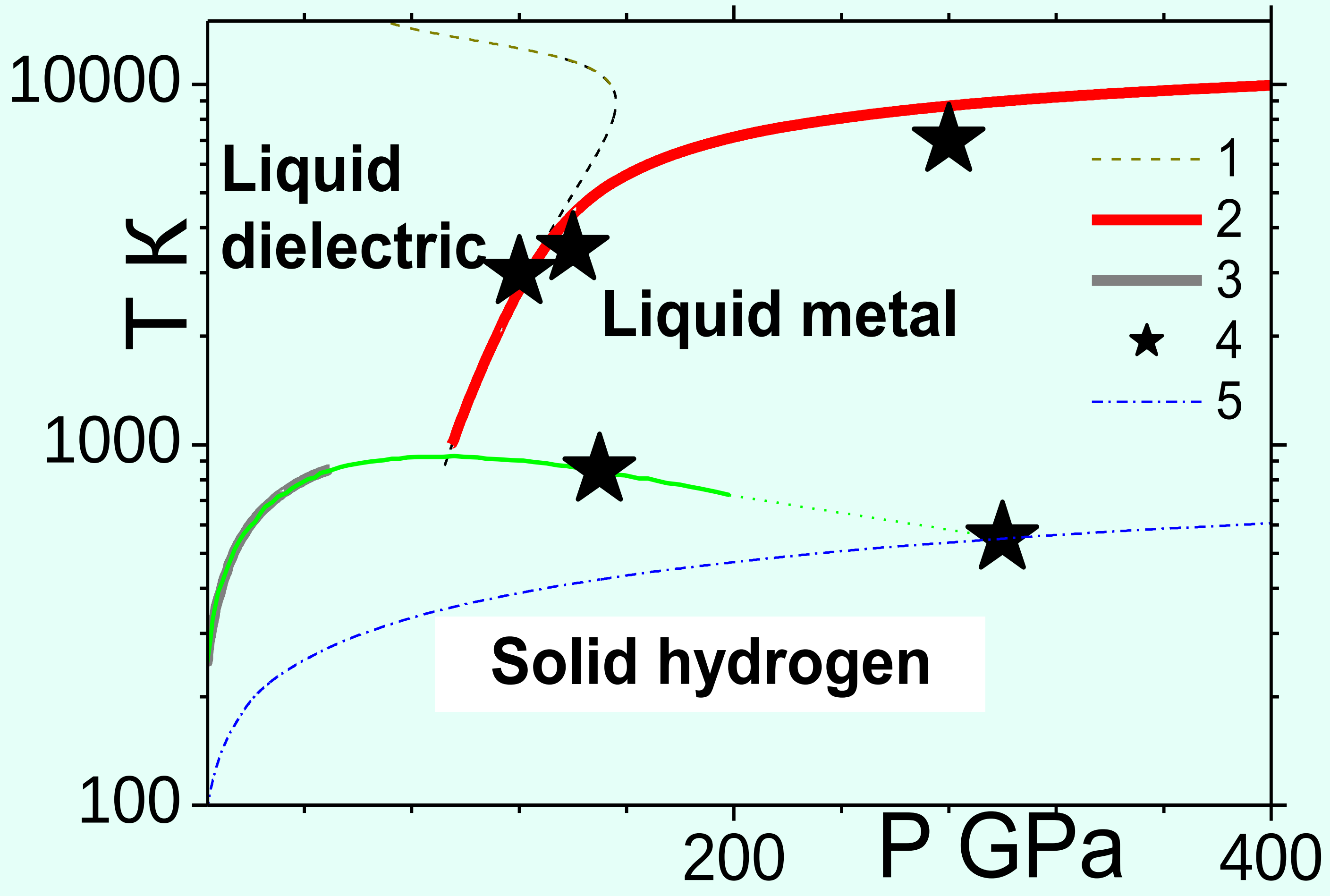
- Semi-empirical equations of state for dielectric and plasma phases of liquid hydrogen were constructed.
- Equilibrium line of plasma phase transition was built. For quasi-isentropic compression, according to the current model, plasma phase transition occurs at the pressure 130 GPa.
- Model reproduces the experimental results for anomalous compressibility and conductivity of hydrogen under assumption that plasma phase clusters are formed in the dielectric phase of hydrogen.

P-T diagram of hydrogen.



Equation of State for liquid

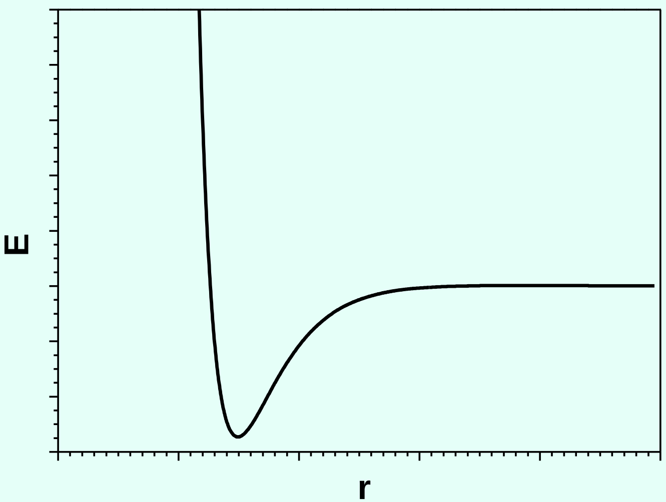
Free energy in fluid variation model

$$F_{liq}(N,V,T) = F_{id}(N,V,T) + F_{\text{int}}(N,V,T)$$

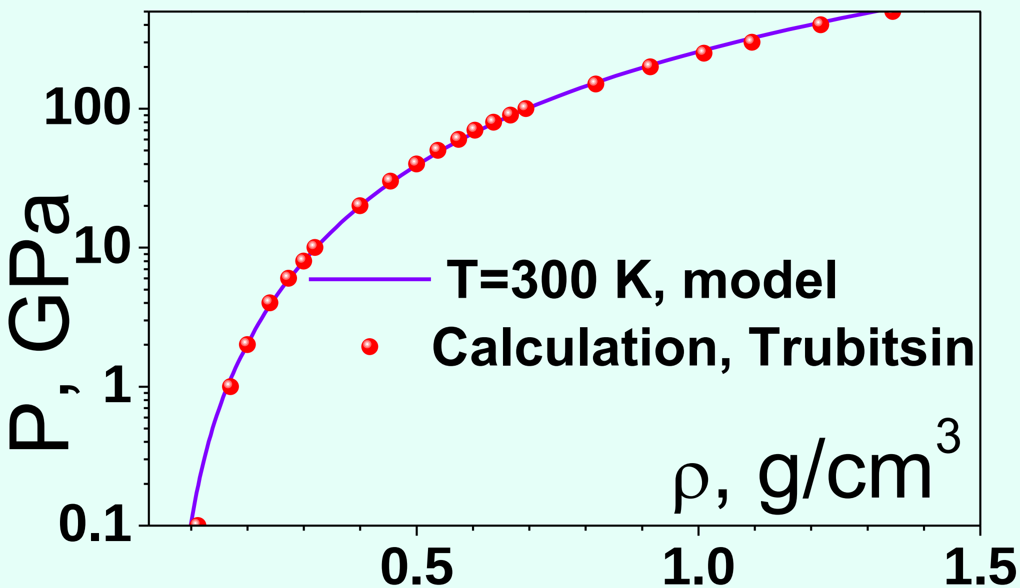
$$F_{\text{int}} = \min_{\eta}\left\{ F^{HS}(\eta) + F^{SS}(\eta)Nk_BT + 12\eta\int_1^{\infty} dx\, x^2 g^{PY}(x,\eta)V(xd) \right\}$$

$$V(r) = \begin{cases} \dfrac{\varepsilon}{\alpha-6}\left[6e^{\alpha\left(1-\frac{r}{r_a}\right)} - \alpha\left(\dfrac{r_a}{r}\right)^6\right], & r > W \\ Ae^{-Br}, & r \le W \end{cases}$$

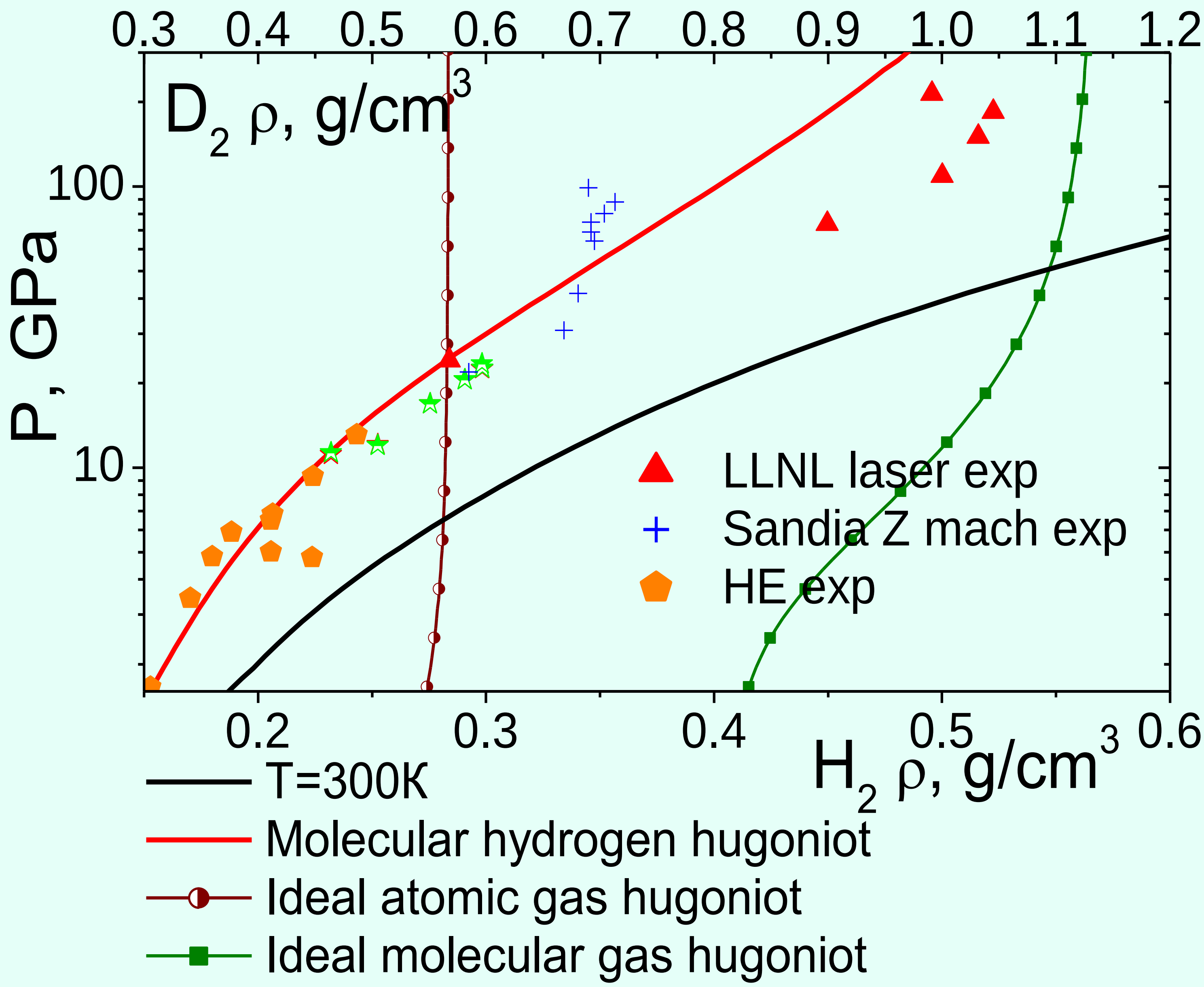
Interaction potential



Isotherm T = 300K of hydrogen



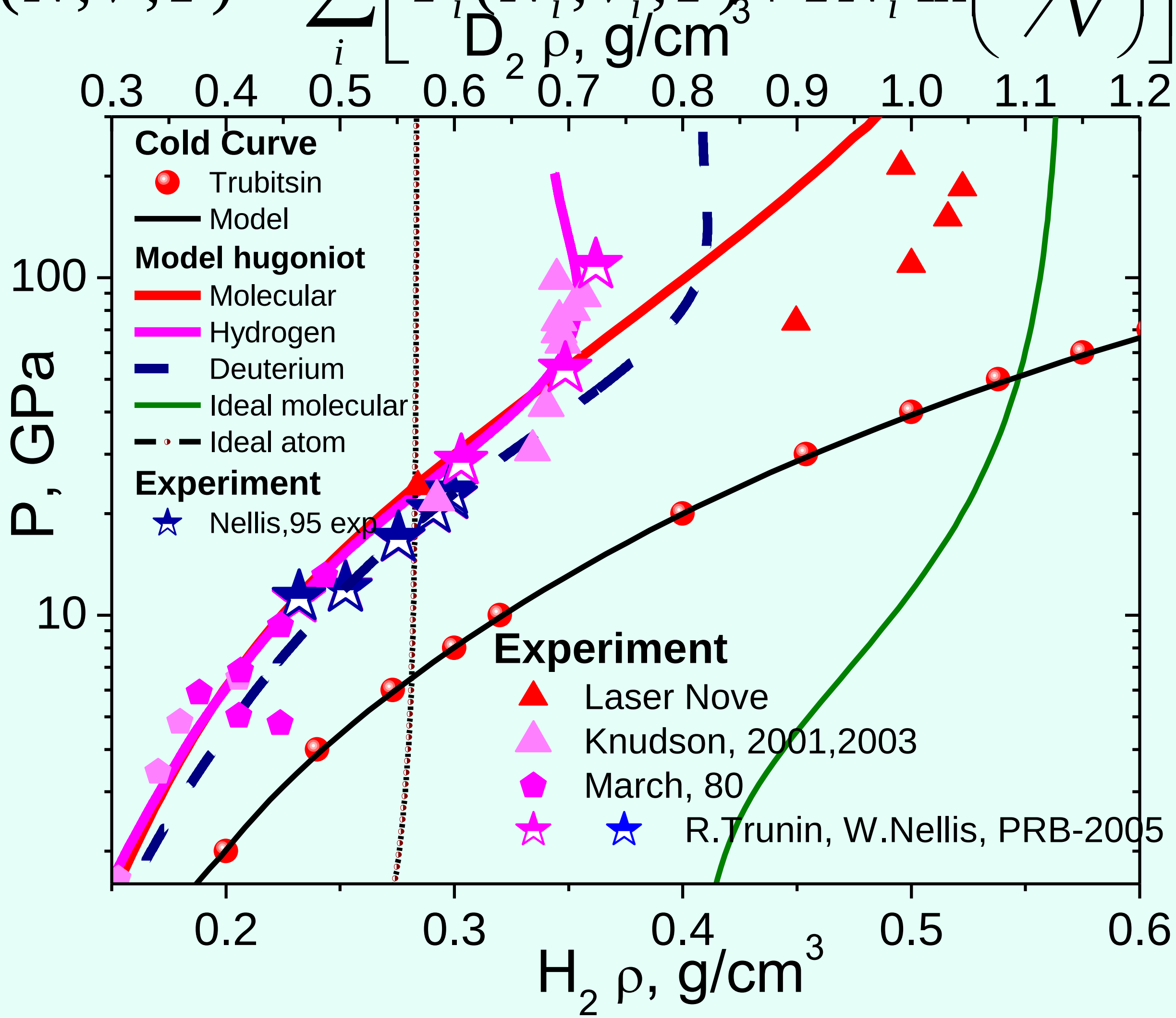
Molecular hydrogen hugoniot



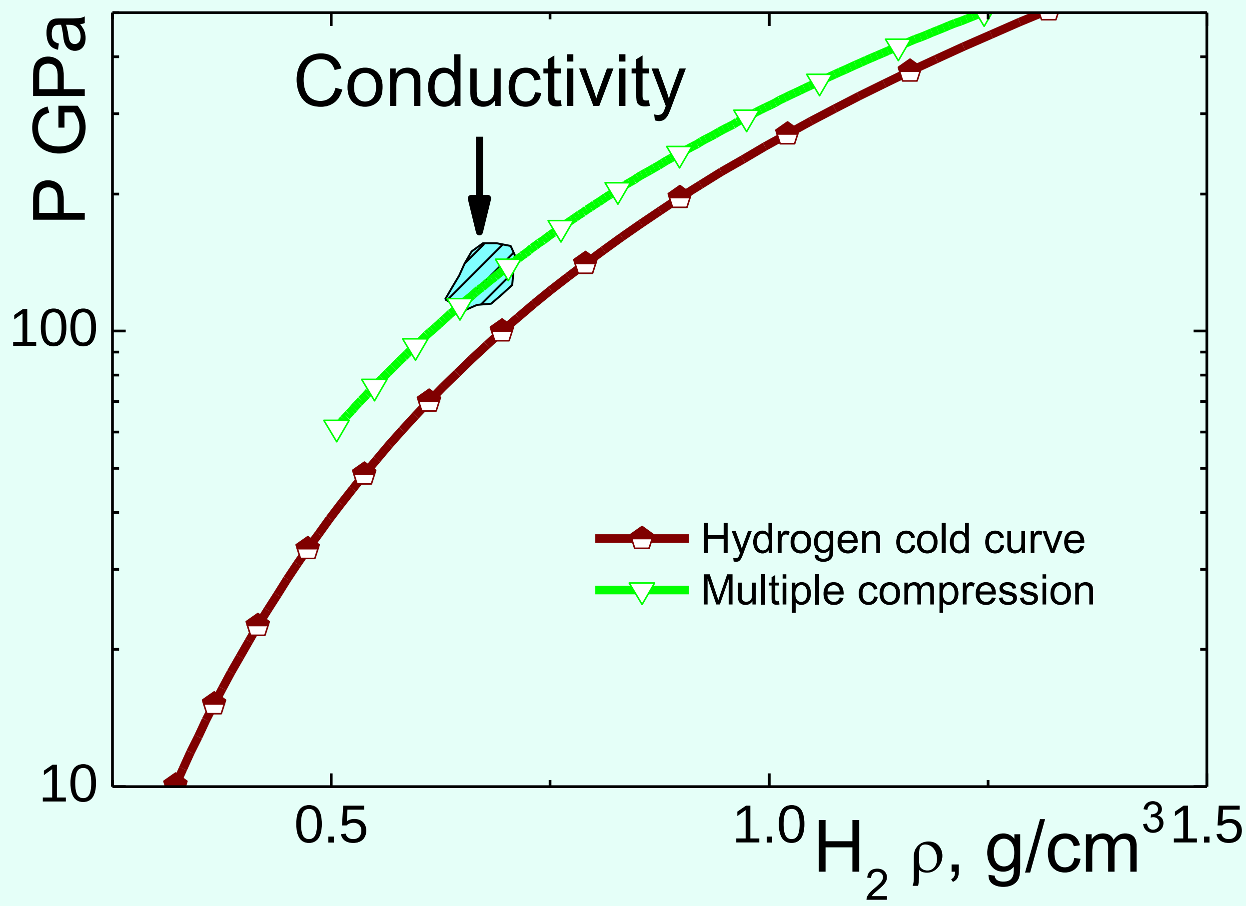
Dissosiation

Free energy of dissociating hydrogen

$$F_{dis}(\vec{N},V,T)=\sum_i\left[F_i(N_i,V_i,T)+TN_i\ln\left(V_i/V\right)\right]$$



Hydrogen isoentropic compression

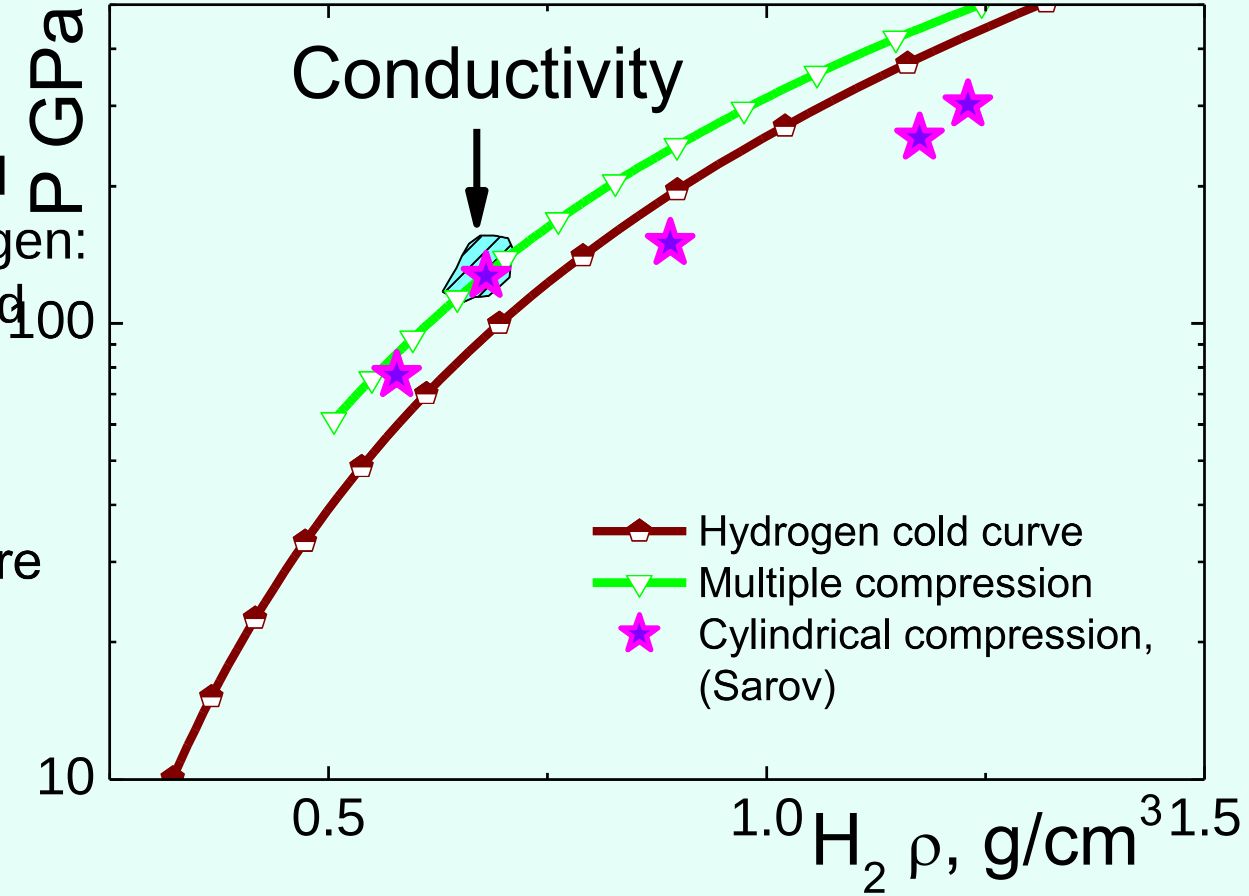


Conductivity reaches maximum value in the region with dissociation ~0.1-1%.

Hydrogen isoentropic compression

In the experiments (Sarov) with cylindrical compression of hydrogen: density larger then cold curve density was registered.

Let's suppose that there exist a metal (plasma) phase of hydrogen



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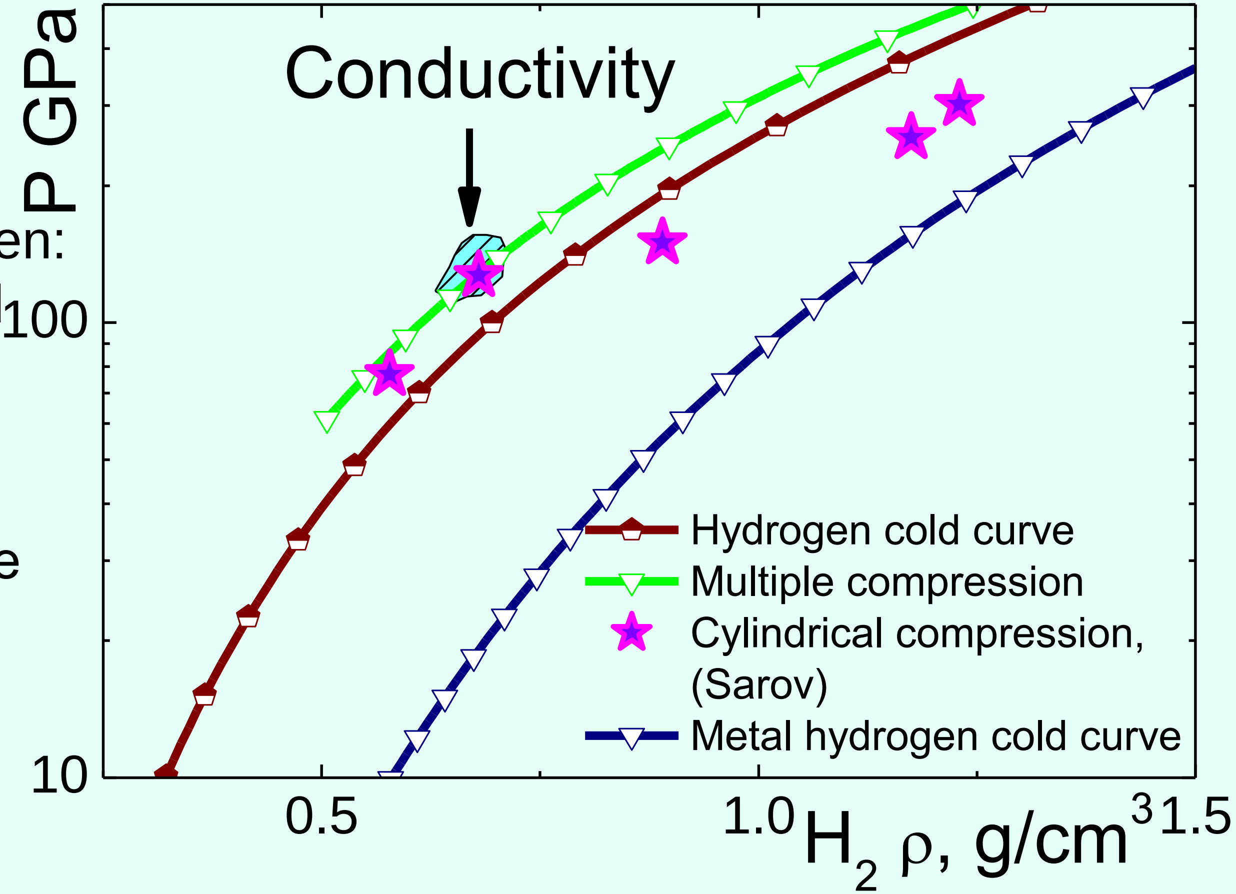
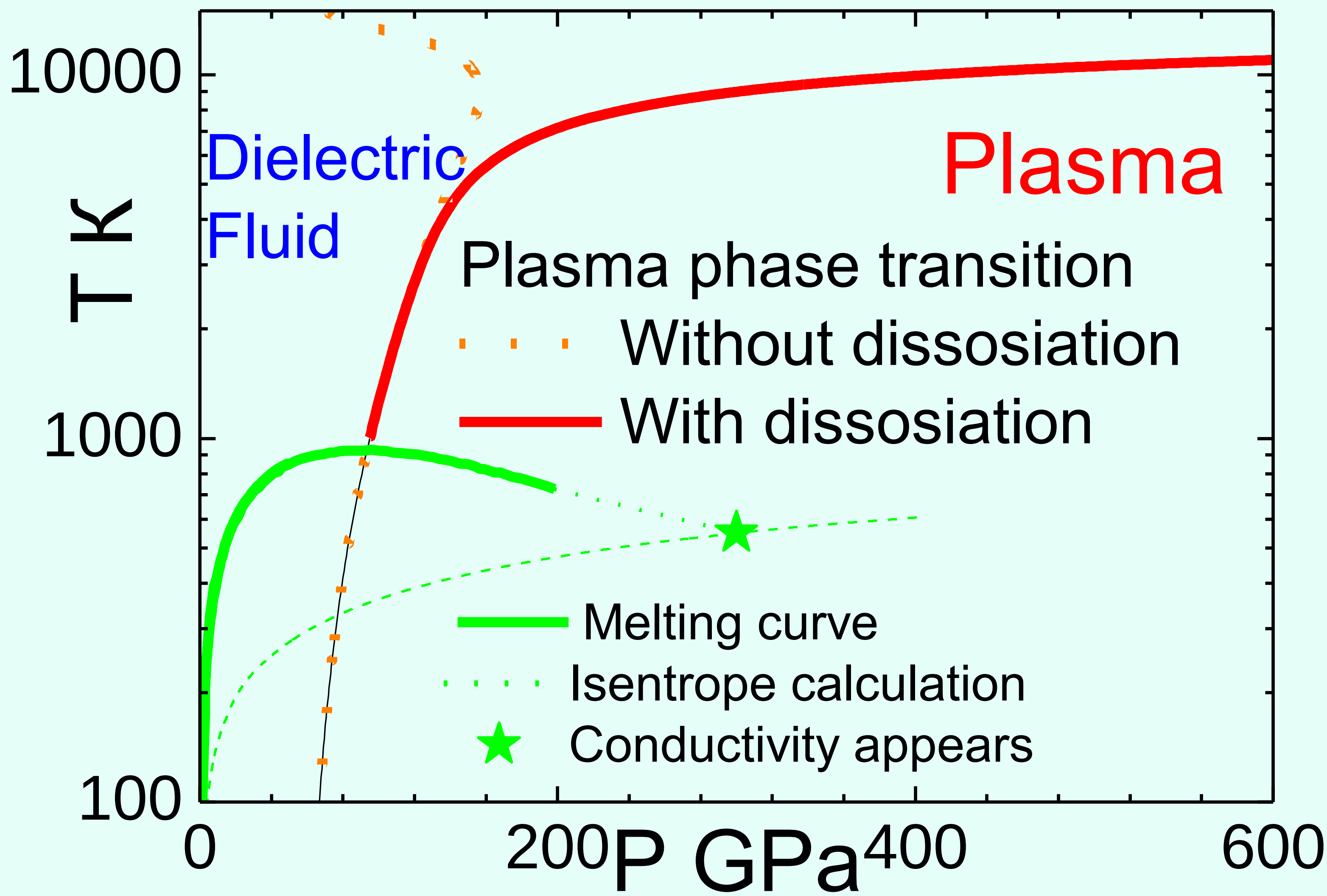


Several theoretical calculations of metal hydrogen cold curve exists.

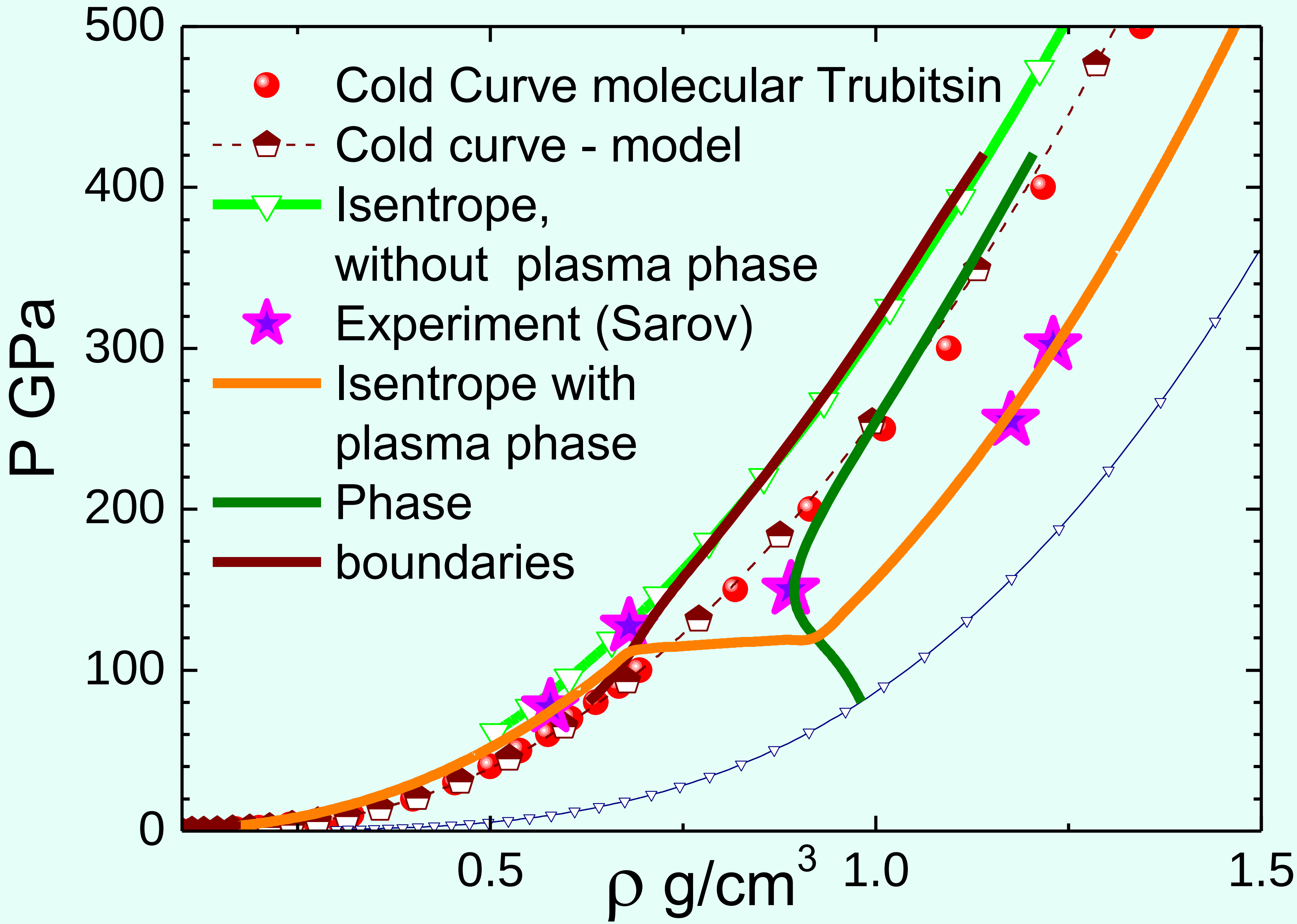
According to them metal hydrogen zero pressure density is ~0.5 g/cm3

For high density cold curve of metal and molecular hydrogen have to be the same.

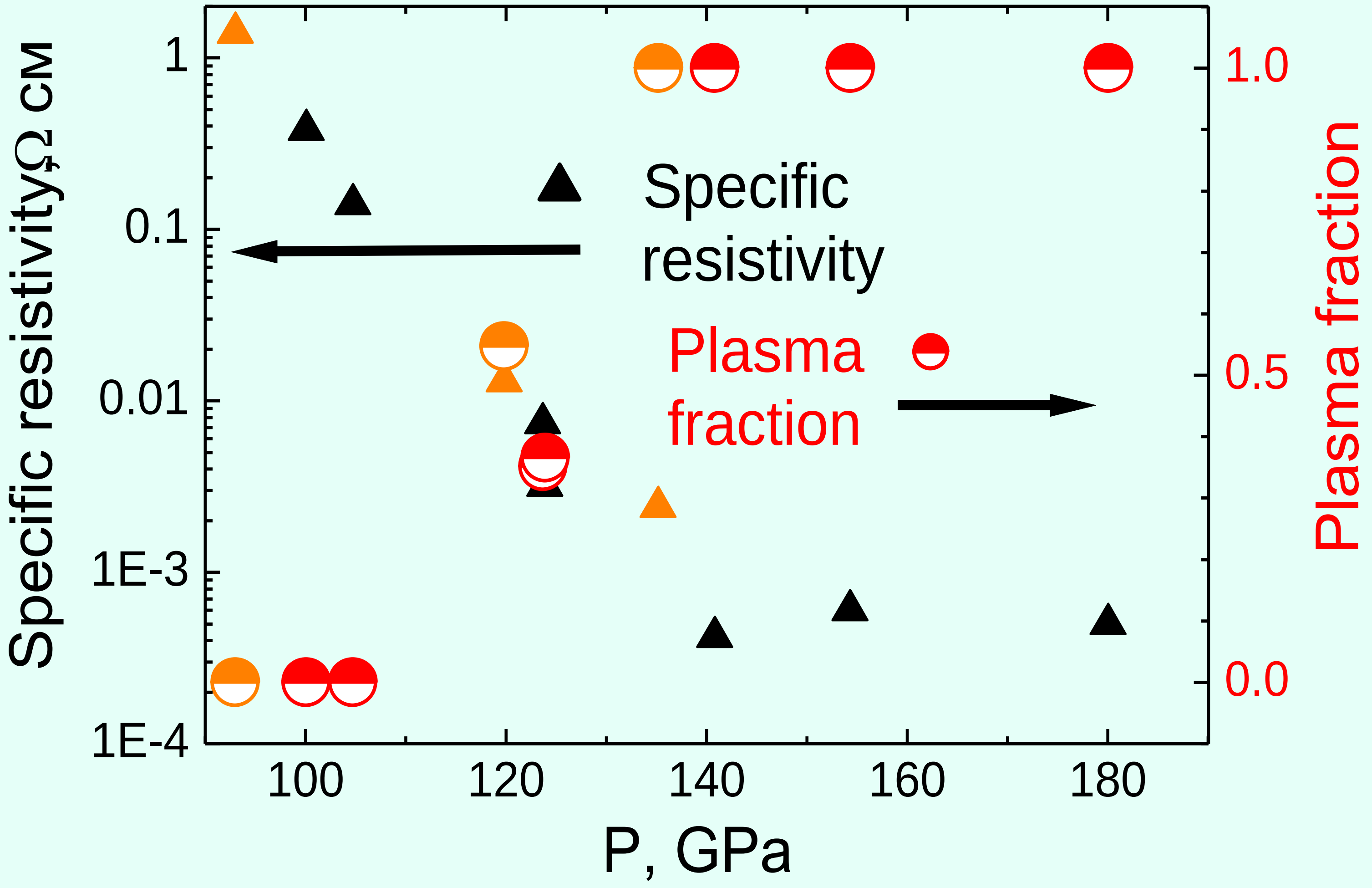
Phase diagram of hydrogen. P-T



Phase diagram of hydrogen. P-ρ



Specific resistivity, mass plasma fraction for different final pressures



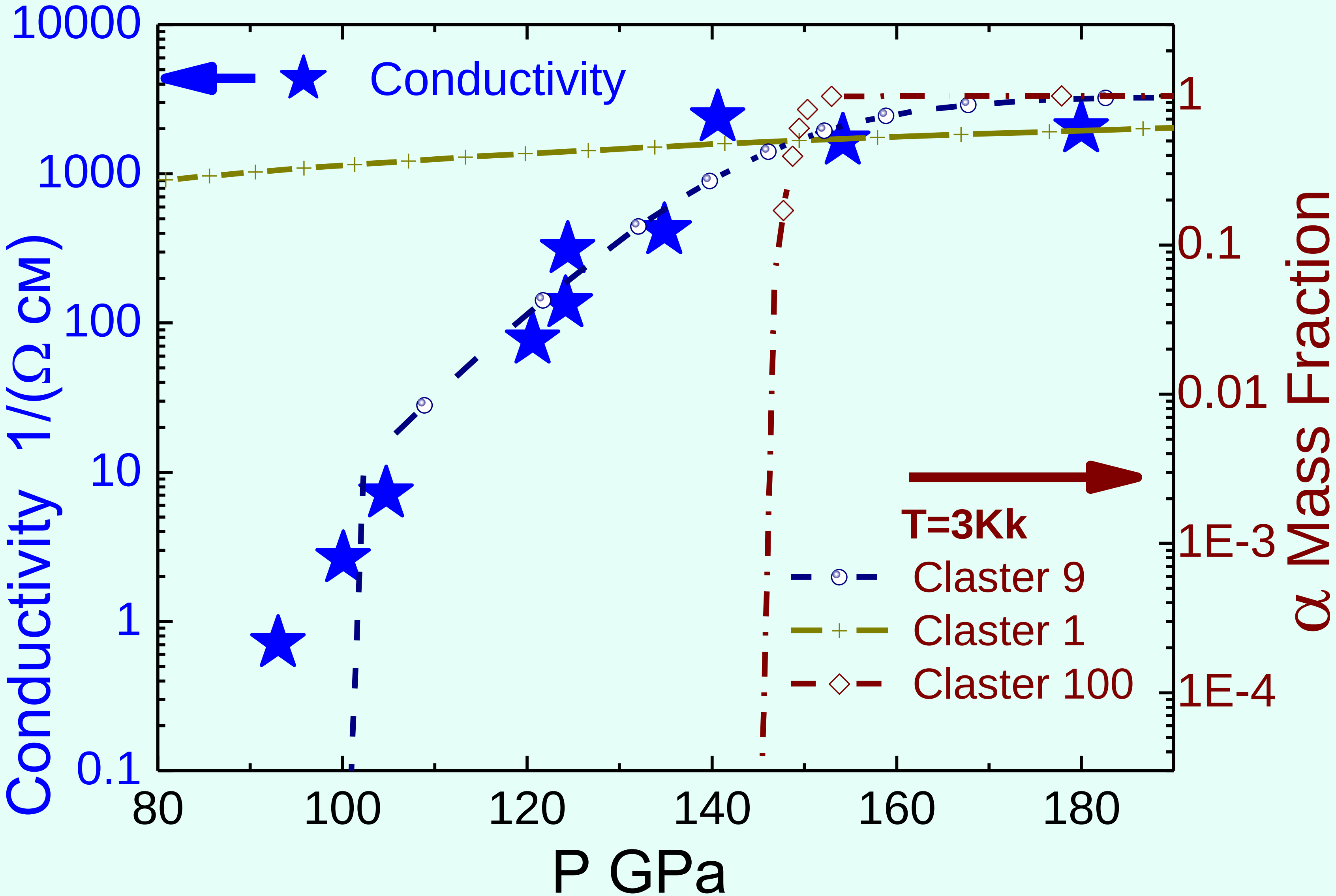
Taking into account hydrogen clusters

A model was used, that finite size cluster formation leads to decreasing of mixture entropy, shifting of energy levels of states.
So, free energy of hydrogen, taking into account cluster formation was taken as modified free energy of dissociating hydrogen.

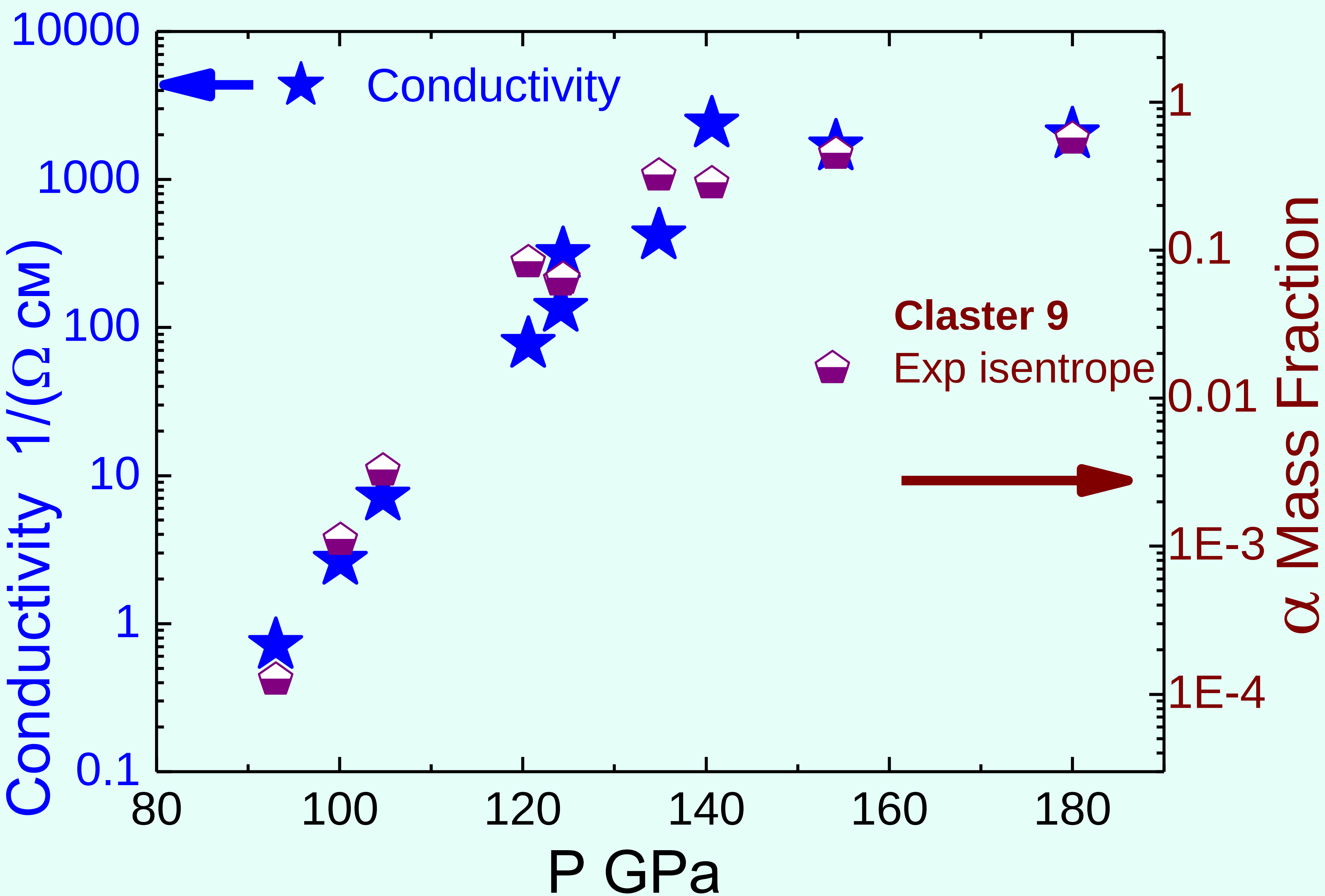
$$F_{clust}(\vec{N},V,T)=\sum_i\left[F_i(N_i,V_i,T)+\frac{TN_i}{S_i^{clust}}\ln\left(V_i/V\right)+N_i\Delta_{S_i^{clust}}\right]$$

where i is dielectric, or plasma fluid.
S_i^{clust} – effective mean size of cluster
$\Delta_{S_i^{clust}}$ - shift of energy of state due to finite mean size of cluster

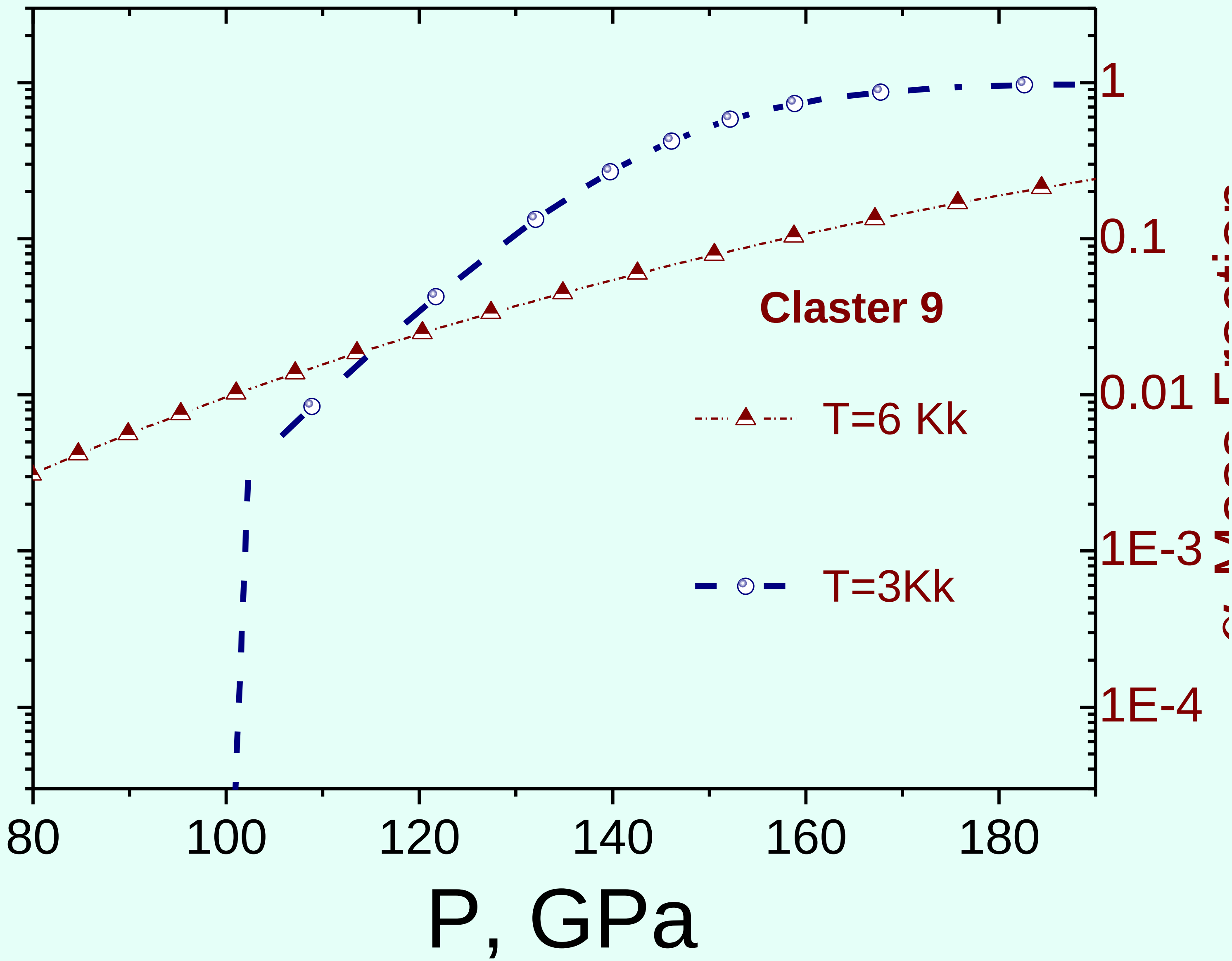
Conductivity for different final pressures. Plasma mass fraction for different cluster sizes



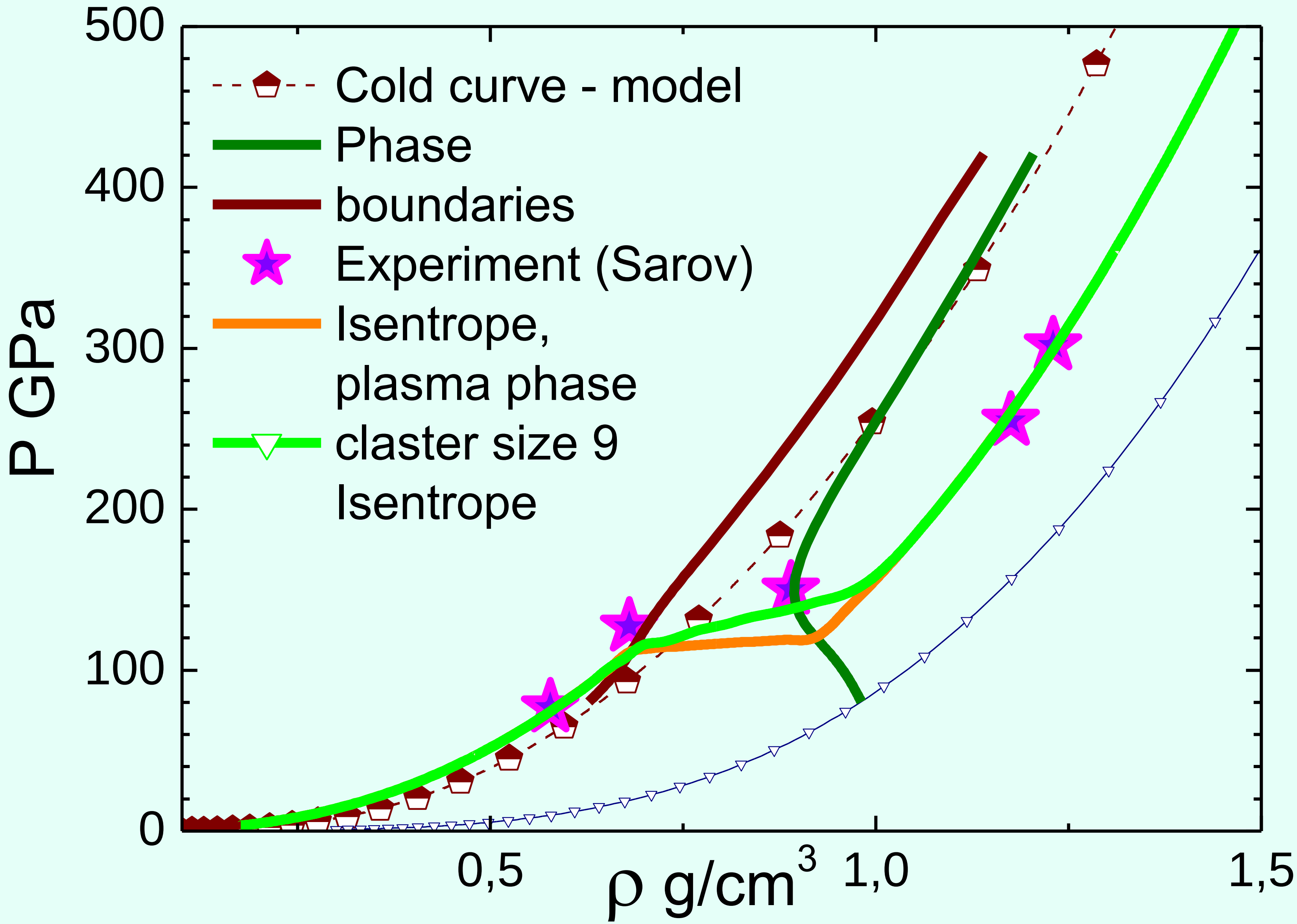
Conductivity for different final pressures. Plasma mass fraction for same PT points



Plasma mass fraction for different temperatures



Phase diagram of hydrogen. P-ρ



Conclusions

1. Semi-empirical multiphase equation of state of hydrogen is constructed. Single shock hugoniot experiments were reproduced in the model of dissociating hydrogen.

2. Plasma phase transition allowed to reproduce experiments with anomalous isentropic compressibility of hydrogen.

3. Conductivity of hydrogen was found proportional to mass fraction of “metal” phase in the plasma cluster model.

4. Model predicts lowering of conductivity with temperature increase from 3000K to 6000K for hydrogen compressed to 130 GPa.