Thermodynamics of shock-compressed hydrogen plasma of megabar pressure range

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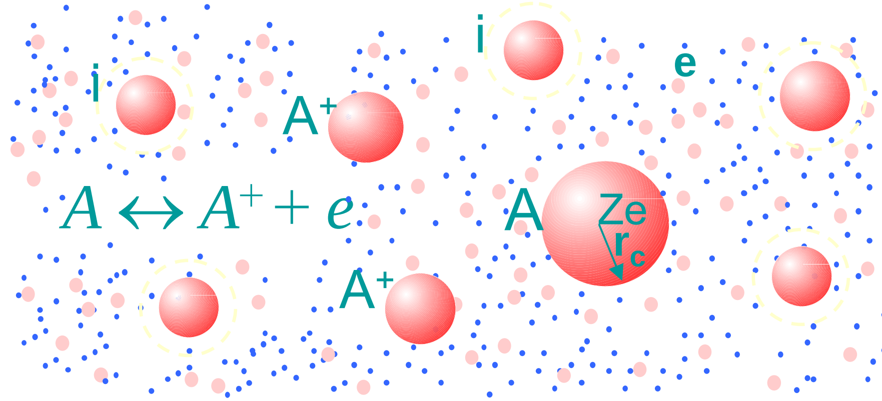
Chemical picture. SAHA-D model

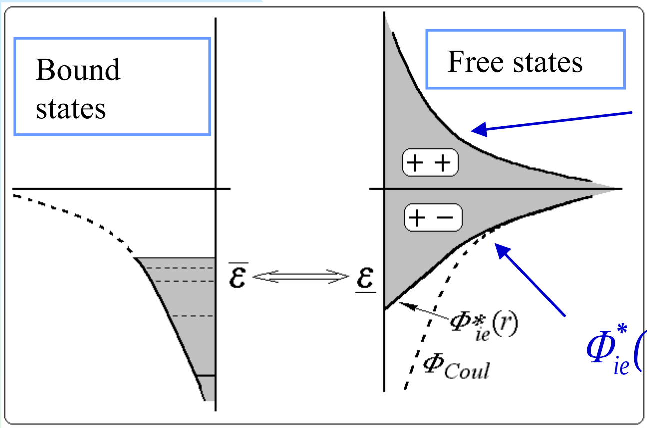
Basic features

- Matter is considered as interacted mixture of atoms, molecules, ions and electrons (H, H2, H+, H2+, e-)
- Coulomb interaction of charged particles – modified pseudopotential model for multi–stage ionization (I.Iosilevskiy)
- Intensive sort-range repulsion - modified soft sphere model (D.Young)
- Electrons are partially degenerated
- Short range attraction (V.Gryaznov, V.Fortov, M.Zhernokletov, I.Iosilevskiy et al., JETP, 1998)

SAHA-D model. Coulomb interaction

Pseudopotential model for multi-stage ionization
(I.Iosilevskiy)





$$\Phi^{*}_{\alpha\alpha}(r) = \frac{Z_\alpha Z_\alpha e^2}{r}$$

ion-ion,
electron-electron

$$\Phi^{*}_{ie}(r) = -\frac{Z_i e^2}{r}\left(1 - e^{-r/\sigma_{ie}}\right)$$

electron-ion

Parameters of correlation functions are defined from conditions **valid at any values of coupling parameter Γ_D**

Corrections to thermodynamic values

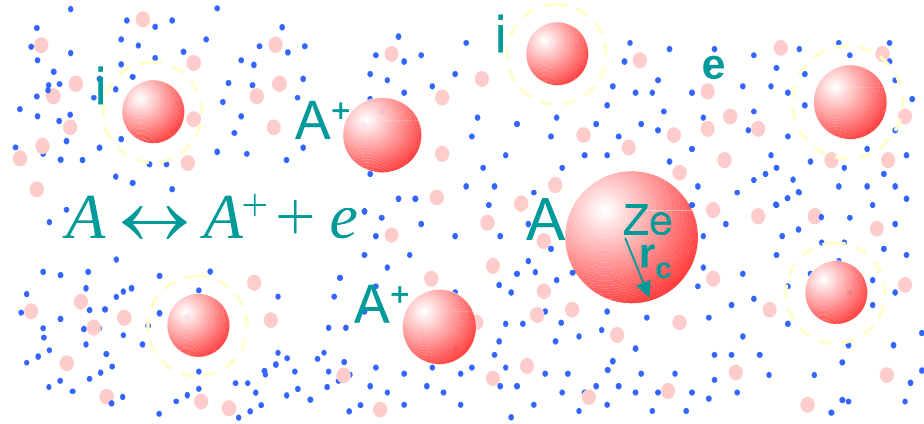
$$\Delta P^{(Coul)}$$

$$\Delta E^{(Coul)}$$

$$\Delta \mu_i^{(Coul)}$$

1. Local electro-neutrality condition
2. ‘Second moment’ conditions of Stillinger & Lowett, (1968)
3. Non-negativity of correlation functions
4. Strong correlation between the ‘depth’ of electron-ionic pseudopotential and amplitude of screening cloud

Saha-D model. Short range repulsion



Short range repulsion:

Modified soft sphere model (D.Young, 1977) for particle mixture of different sizes

$$r_c = \left[\sum n_j r_j^3 / \sum n_j\right]^{1/3}$$

$$\frac{\Delta F_{SS}}{Nk_BT} = C_s y^{s/3}(\varepsilon_{SS}/k_BT) + \frac{s+4}{6} Q y^{s/9}(\varepsilon_{SS}/k_BT)^{1/3};$$

$$y = \frac{3Y\sqrt{2}}{\pi}; \quad Y = \frac{4\pi r_c^3}{3} = \frac{\pi\sigma_c^3}{6}$$

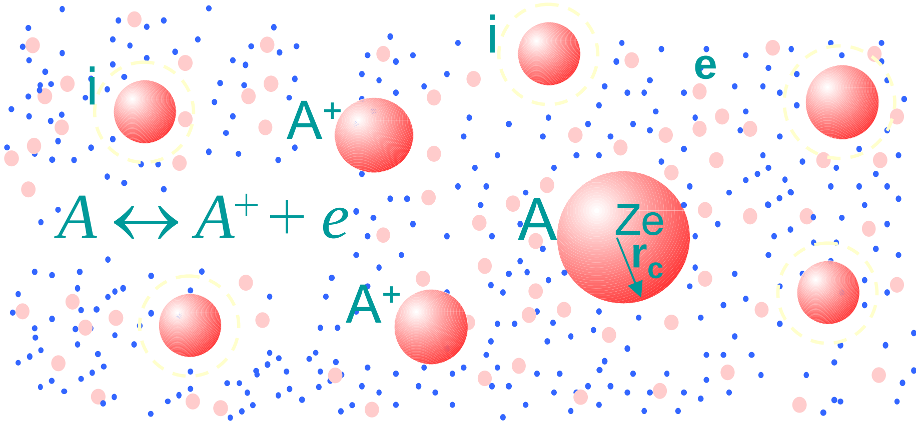
1. Parameters of molecule D_2 (R_M, s, ε_{SS}) and atom D (R_A, s, ε_{SS}) are determined in accordance with non-empirical atom-atom approximation

E.Yakub, *High.Temp*, **28**, (1990), 664

2. Key parameter **R(D) / R(D_2)=0.8**

Saha-D model. Short range attraction

Short range attraction:



$$\Delta F_{mm} = \Delta E_{mm} = -A\left(\sum N_i\right)^{1+\delta} \cdot V^{-\delta}$$

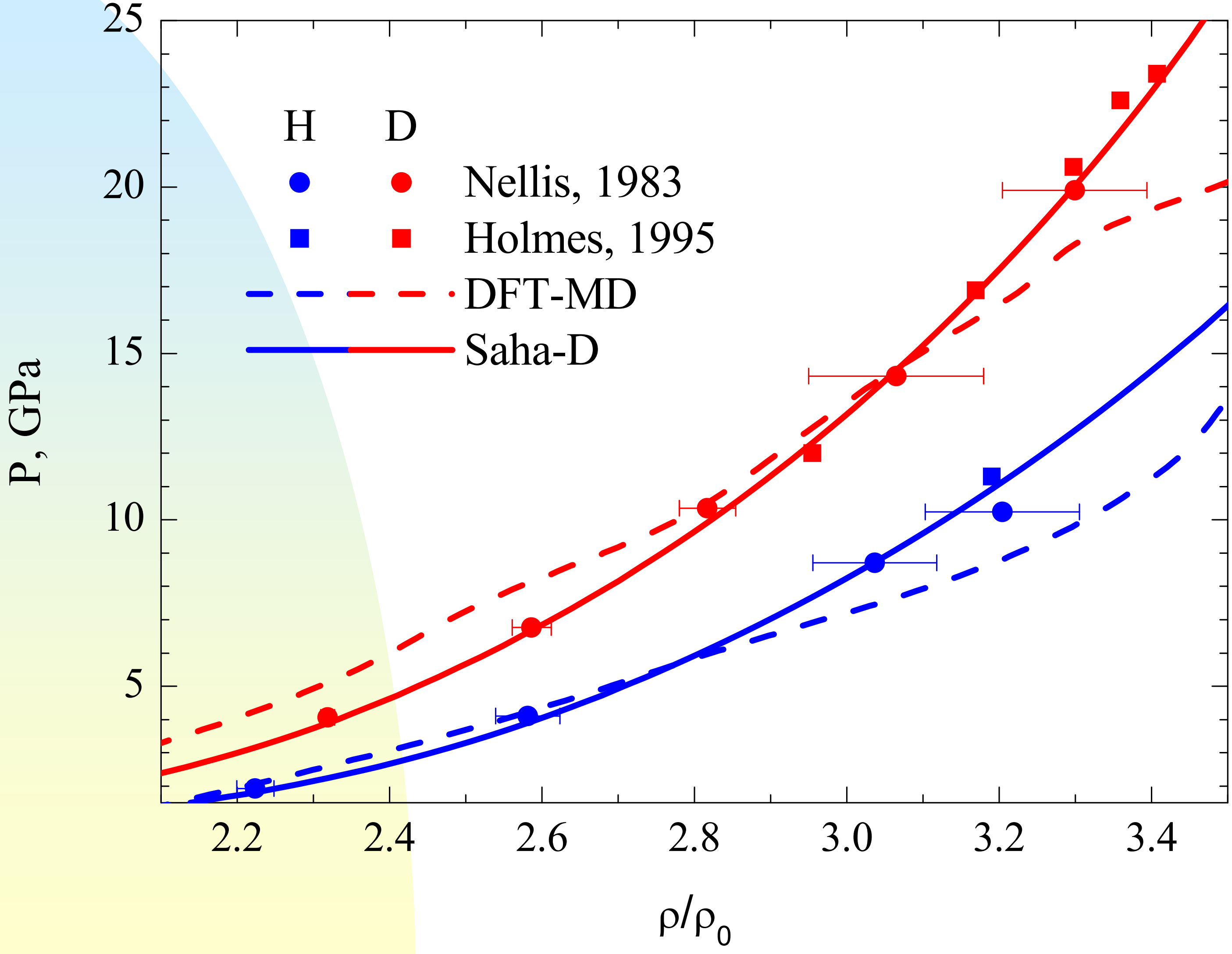
$$\Delta P_{mm} = -A\delta\, V^{1+\delta}; \quad A, \delta = const$$

Attractive corrections are independent of temperature.
δ=*1* – Van der Waals-like approximation.
Parameter *A* supplies correct sublimation energy of molecular system at condensed state

V.Gryaznov, V.Fortov, M.Zhernokletov, I.Iosilevskiy et al, JETP, **87**, (1998), 678

Hugoniots of liquid hydrogen and deuterium

Experimental data and model calculations



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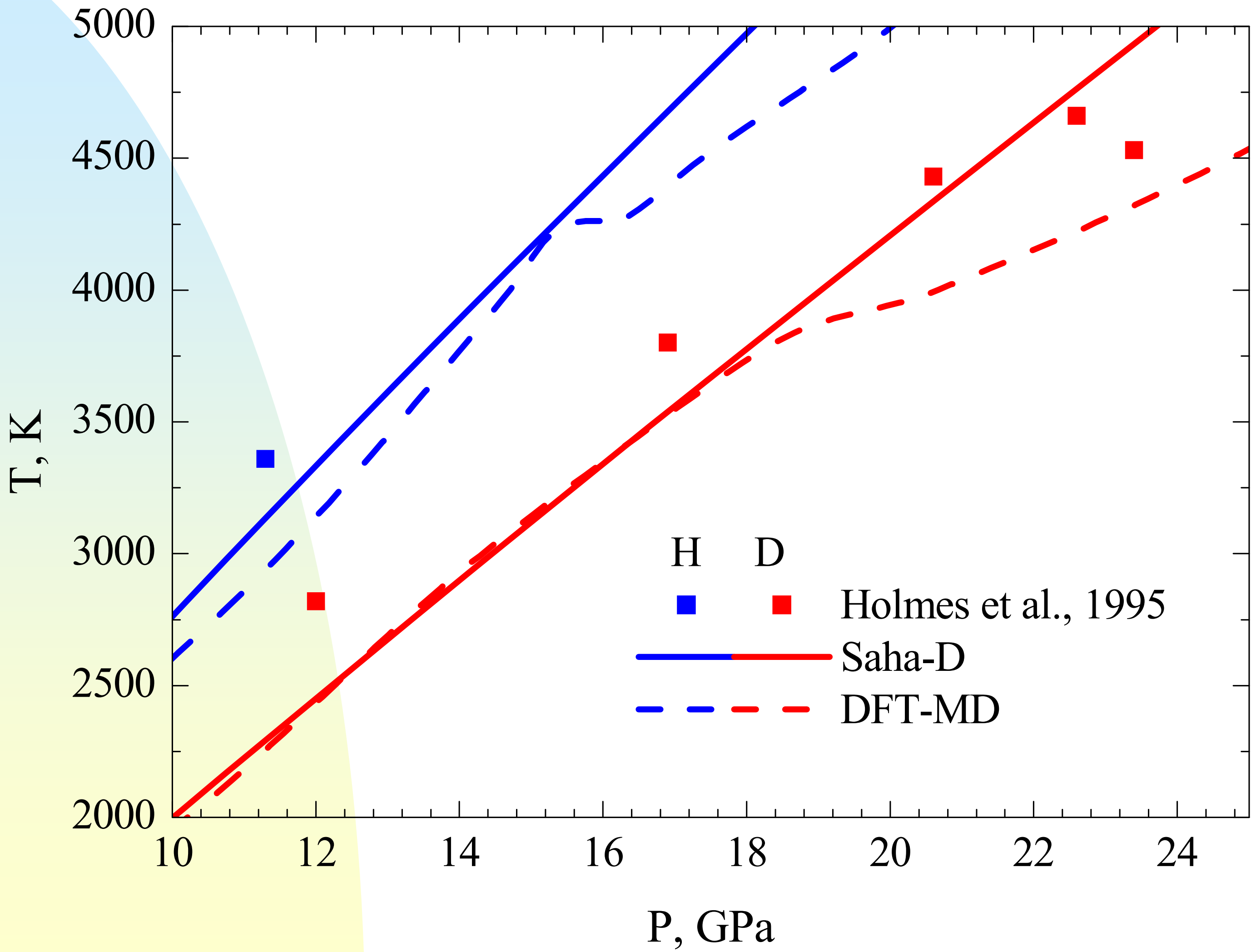
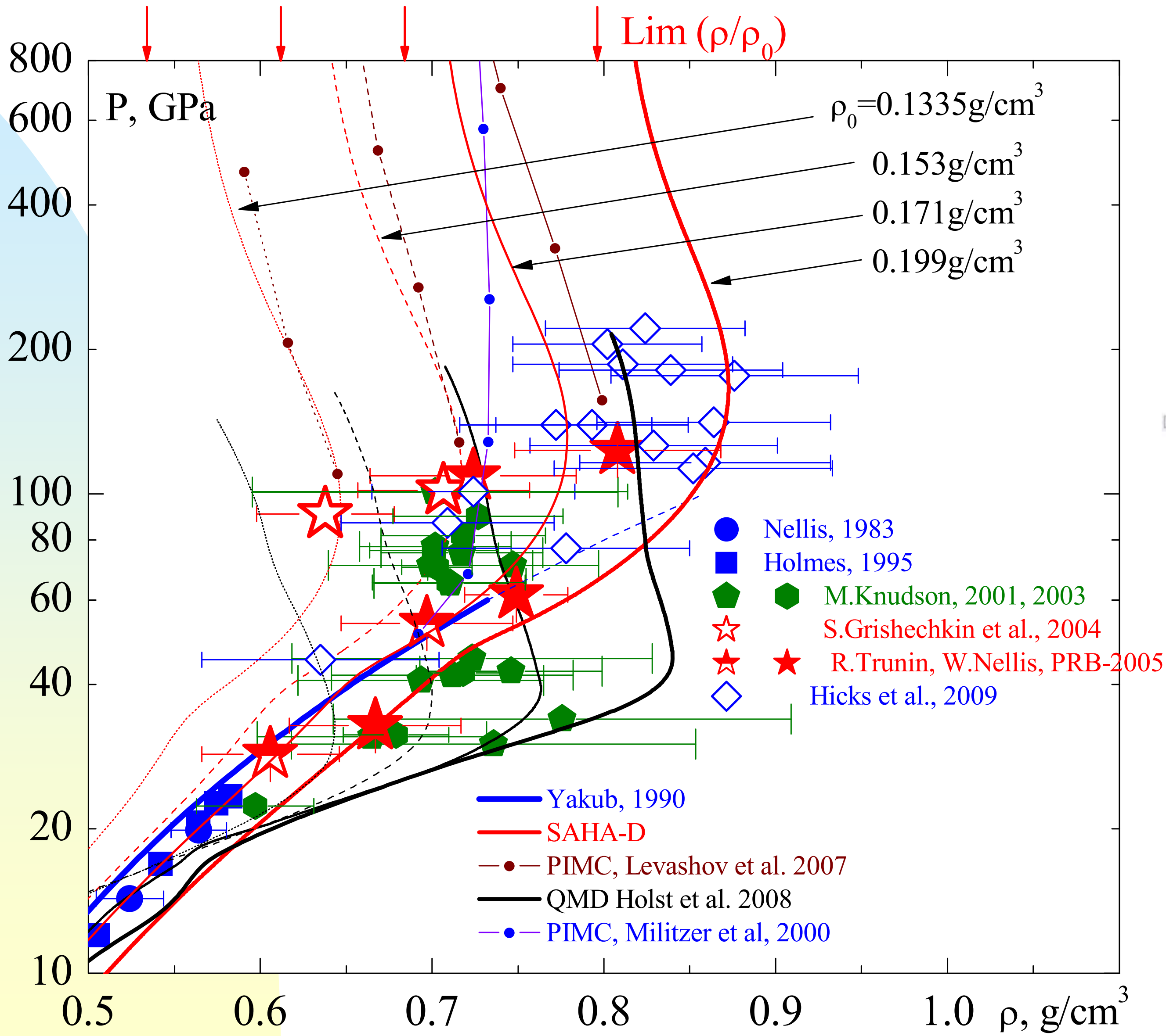


Hugoniots of fluid deuterium

New experimental data and model calculations



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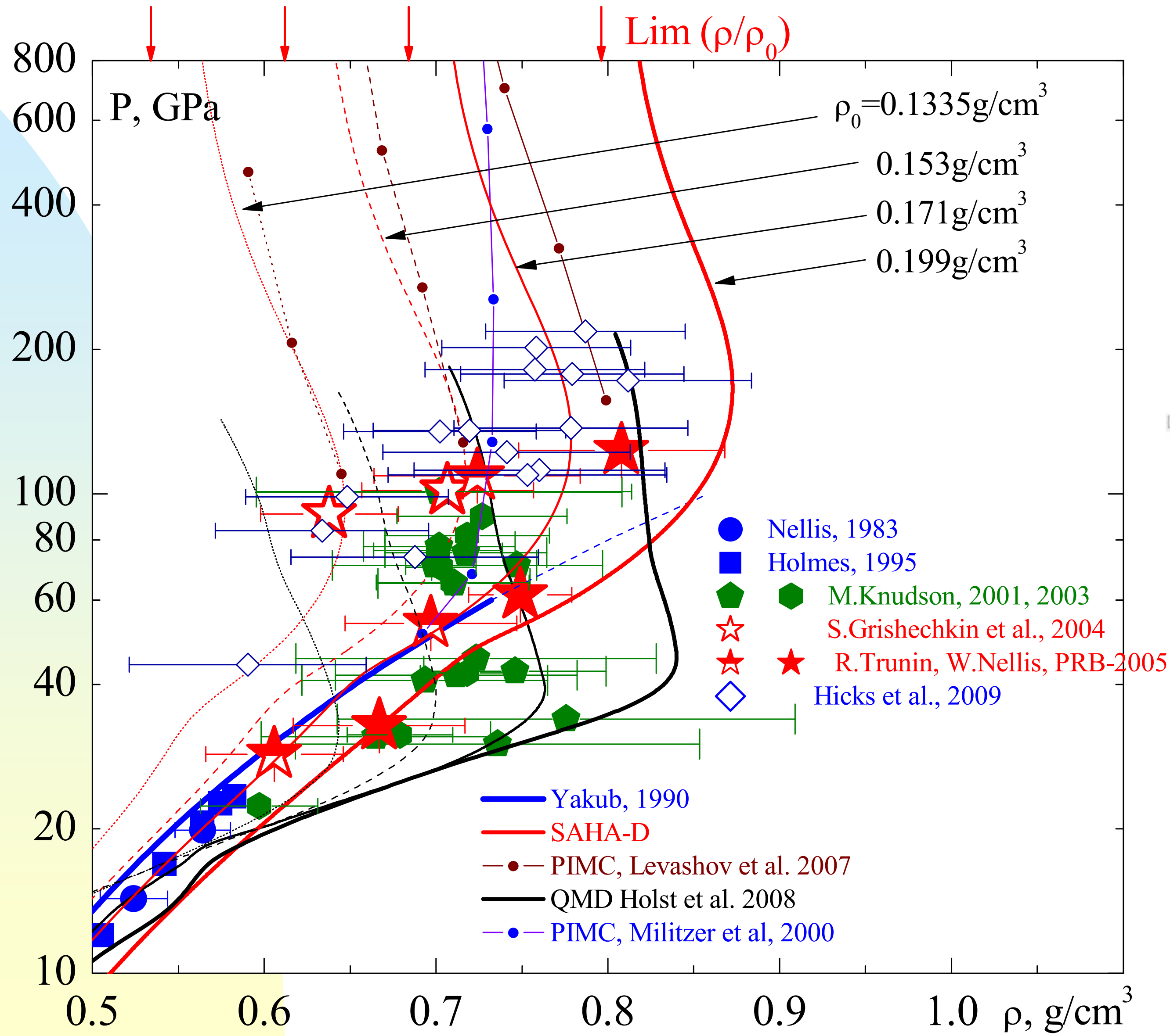

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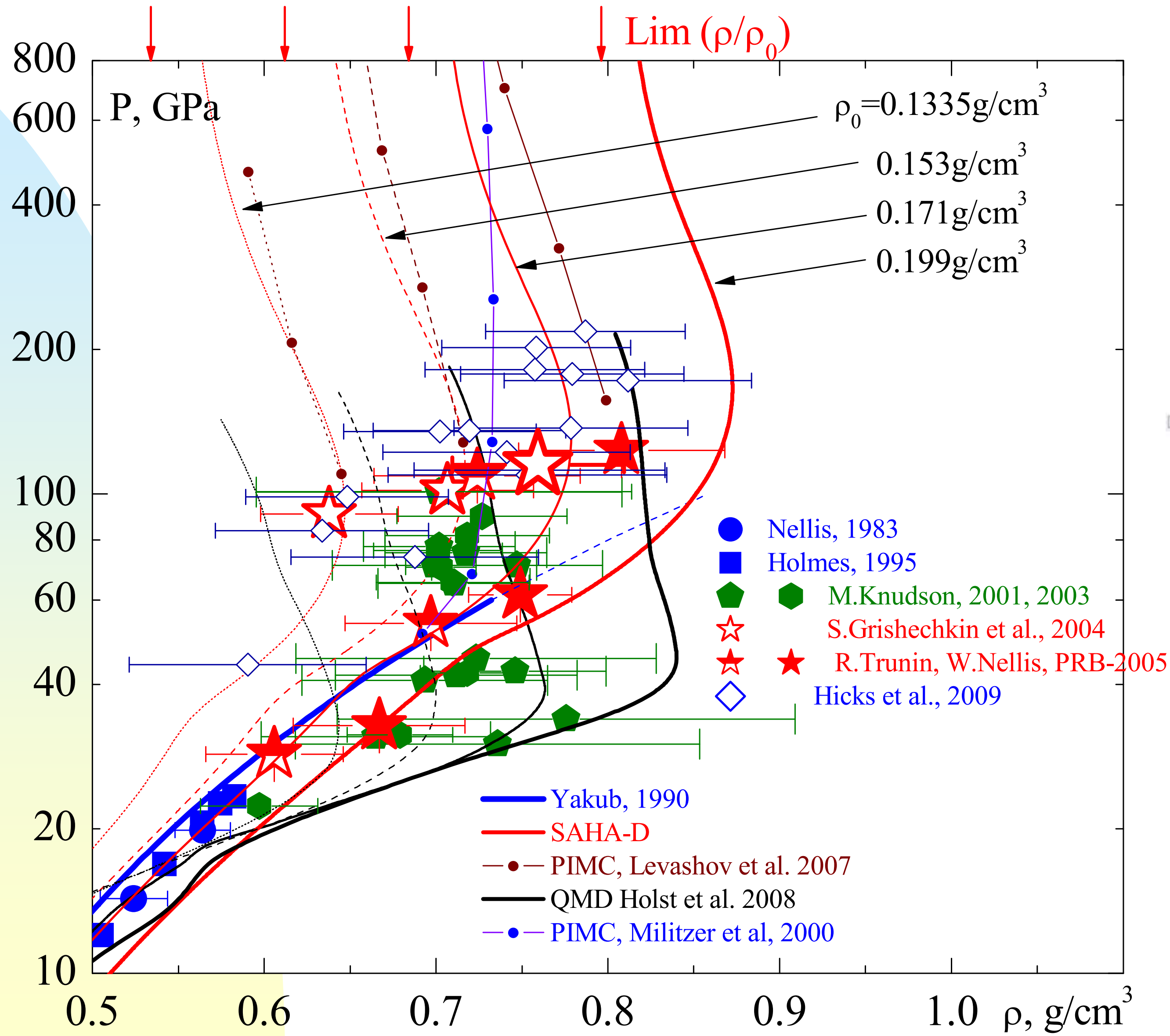
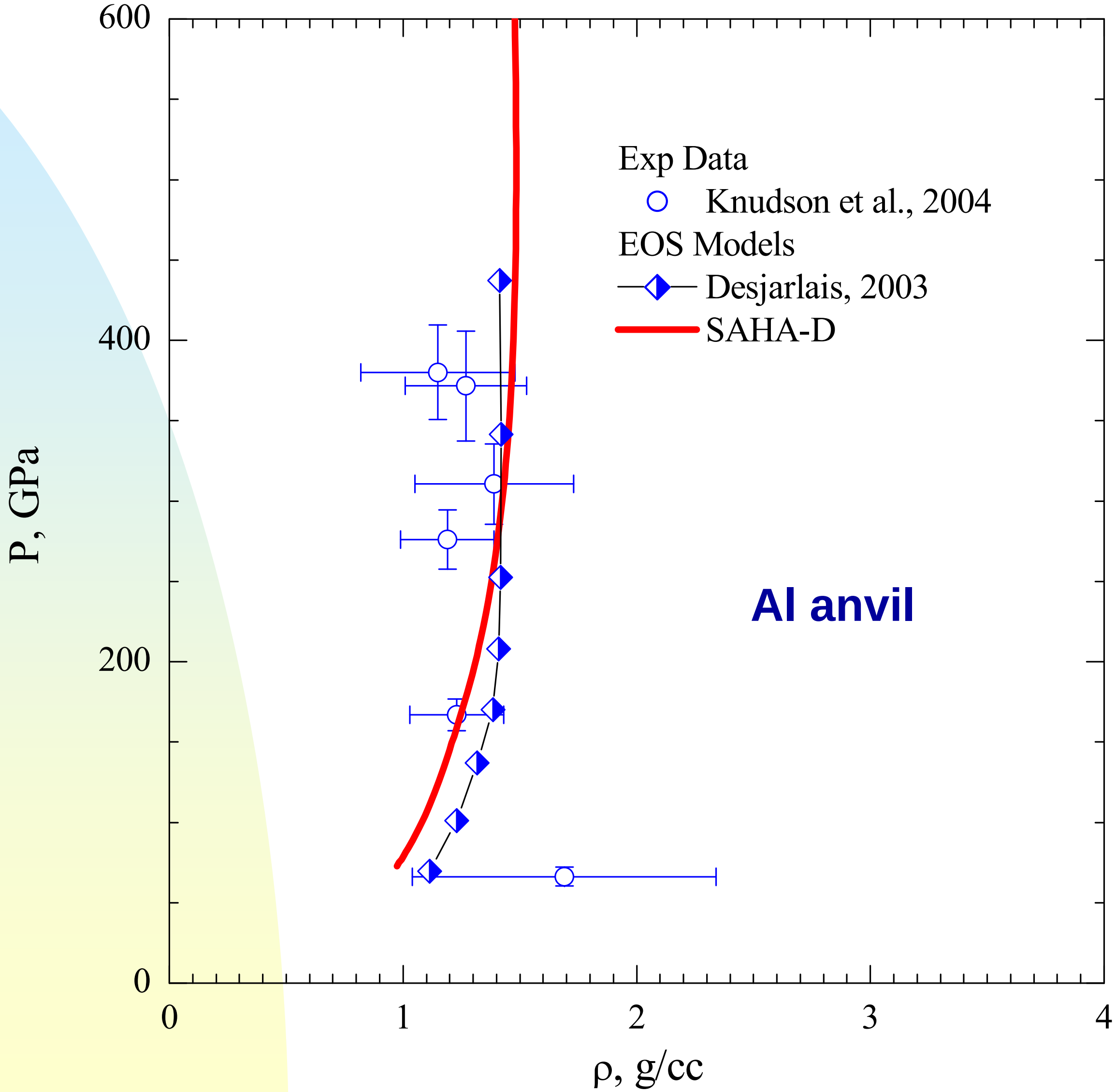


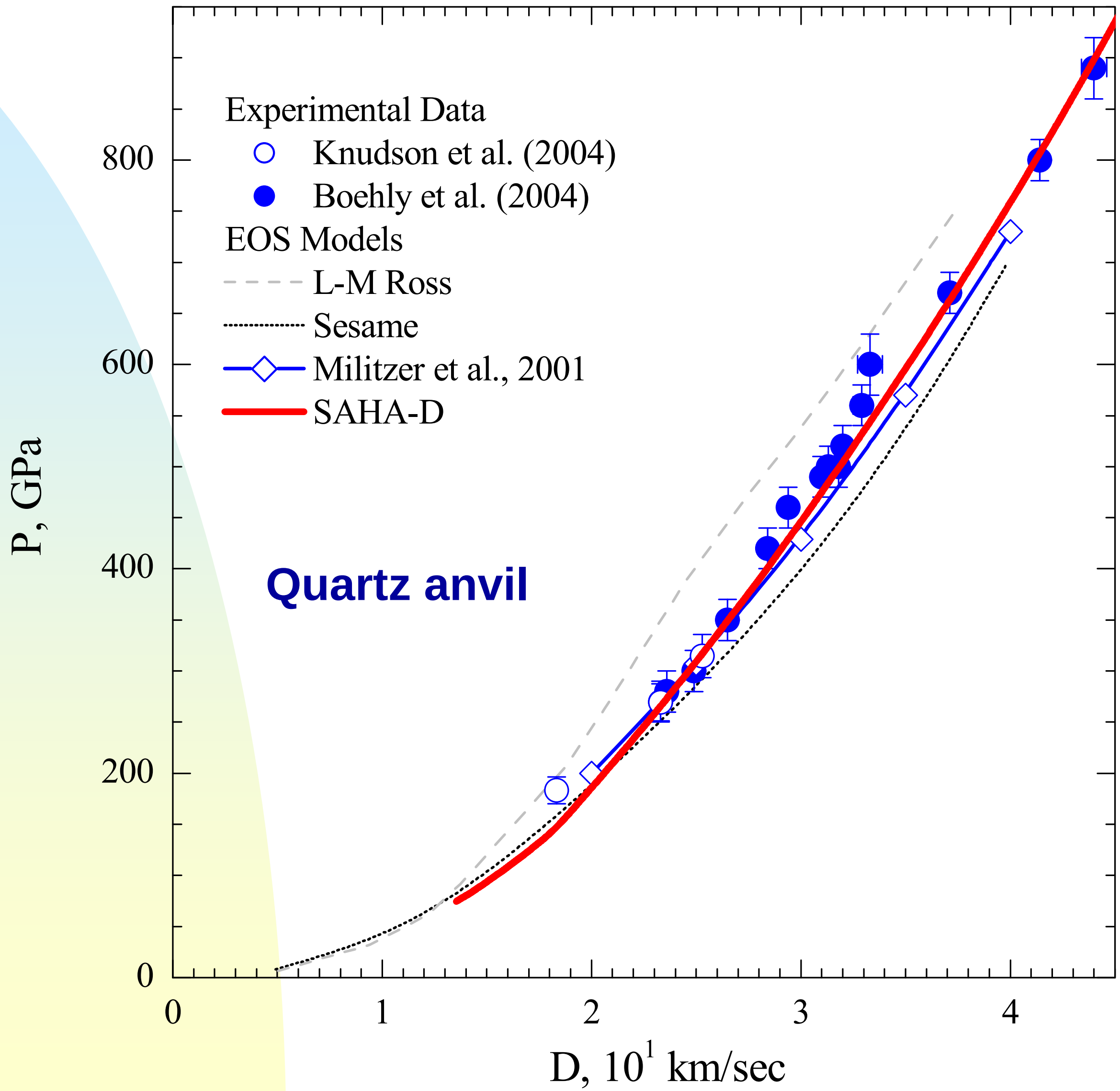
Liquid deuterium. Secondary shock
Experimental data and model calculations



Sandia National Laboratories

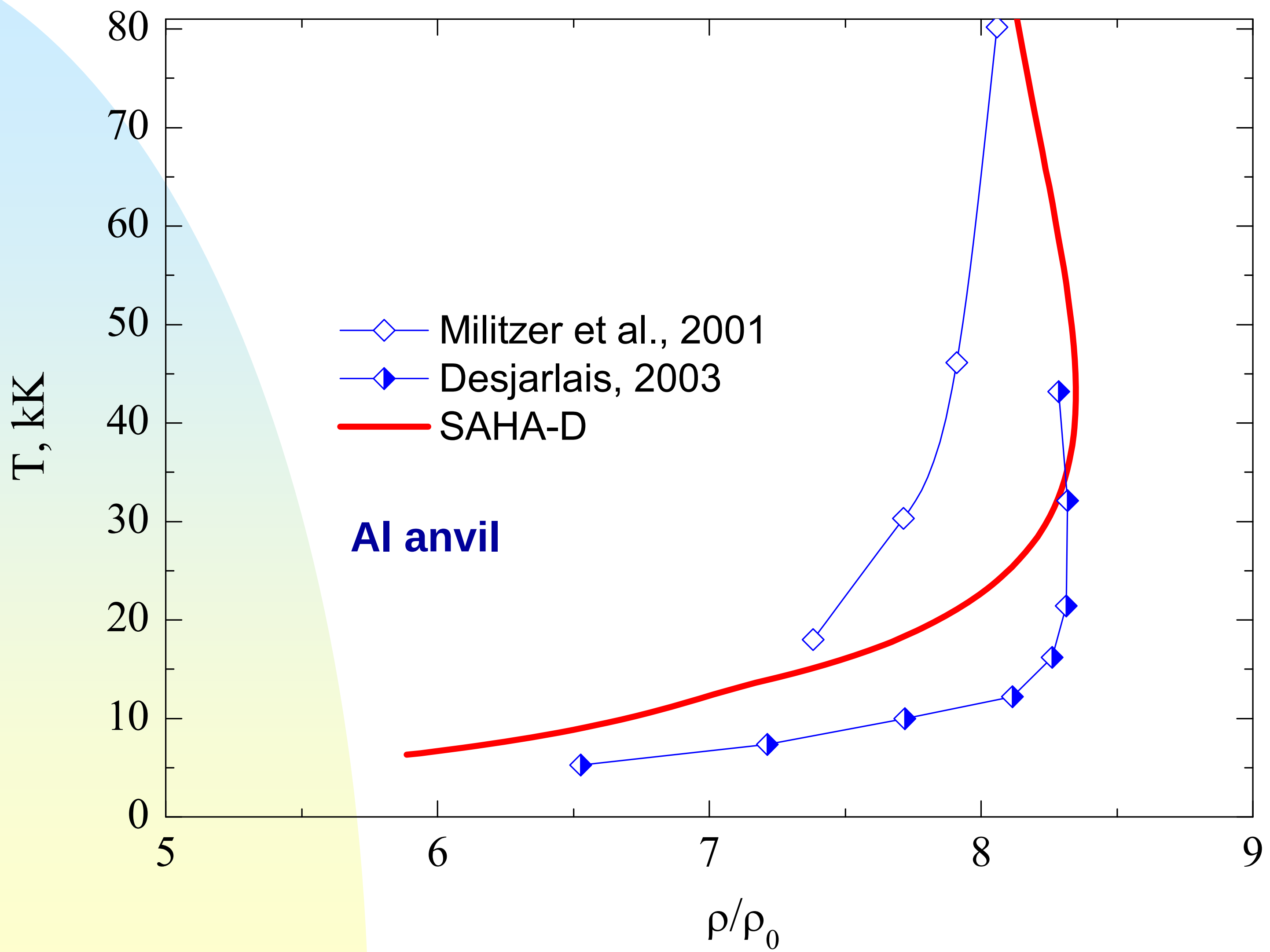
Liquid deuterium. Secondary shock

Experimental data and model calculations

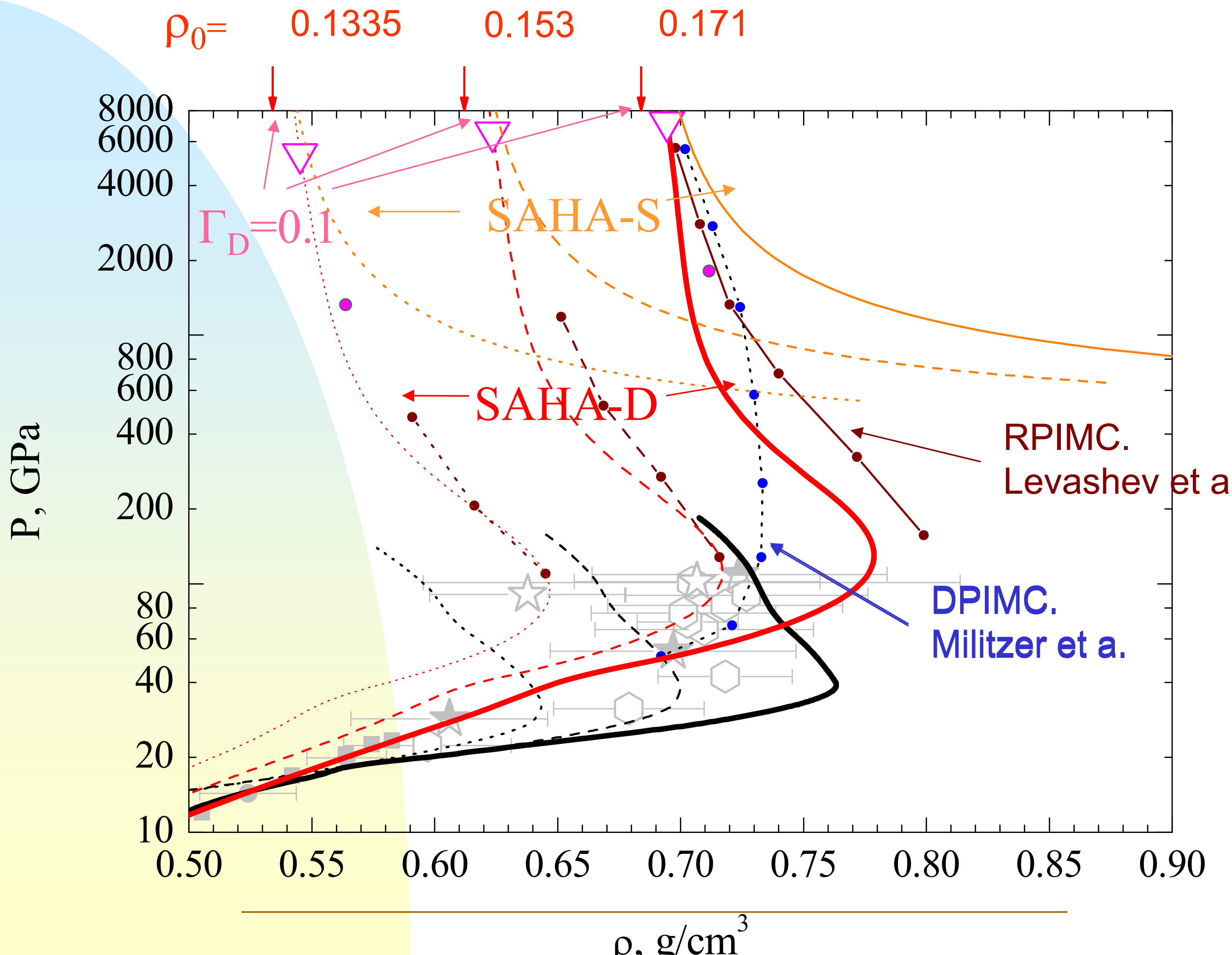


Liquid deuterium. Secondary shock

Model calculations



Validation of high-temperature asympthotics



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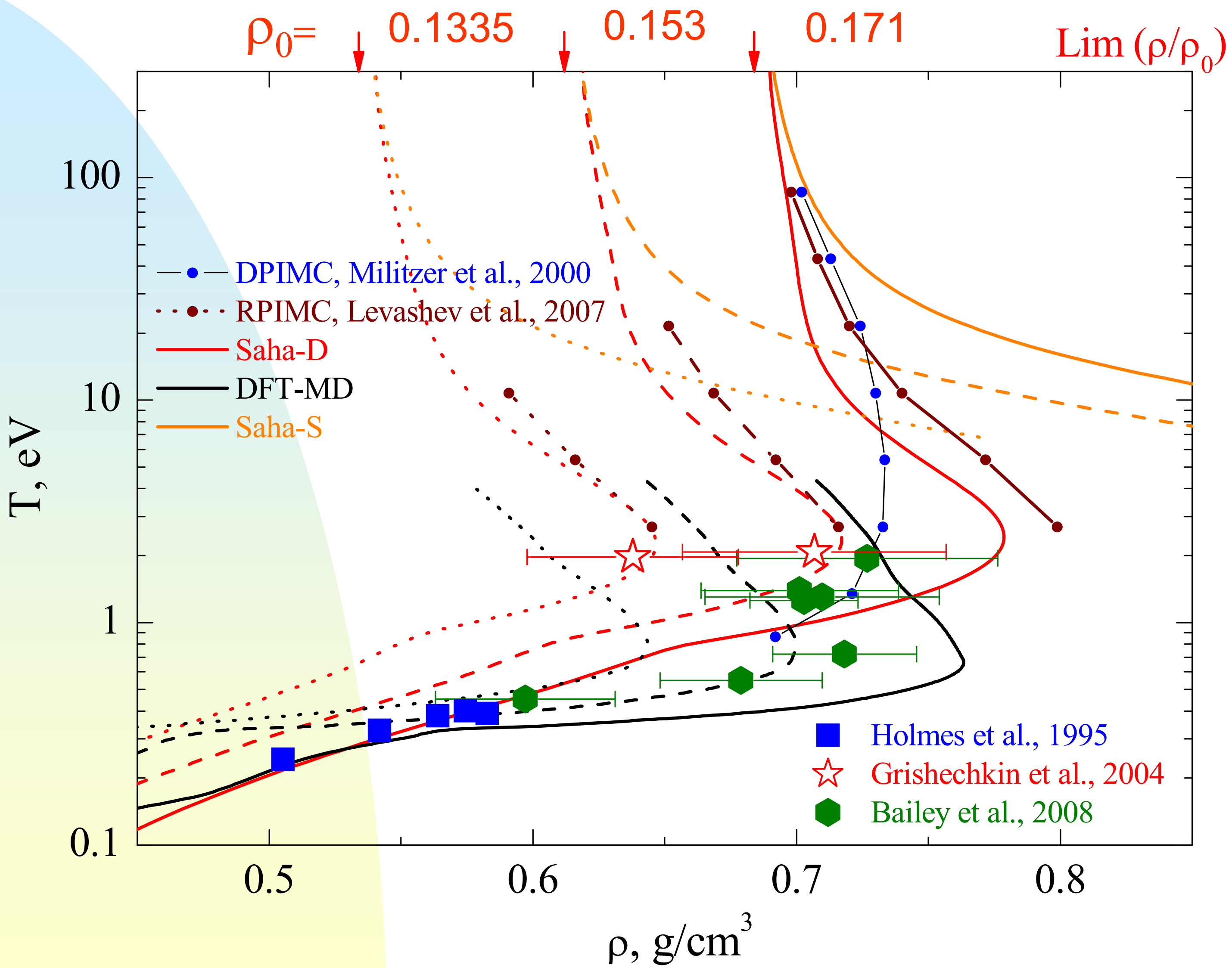

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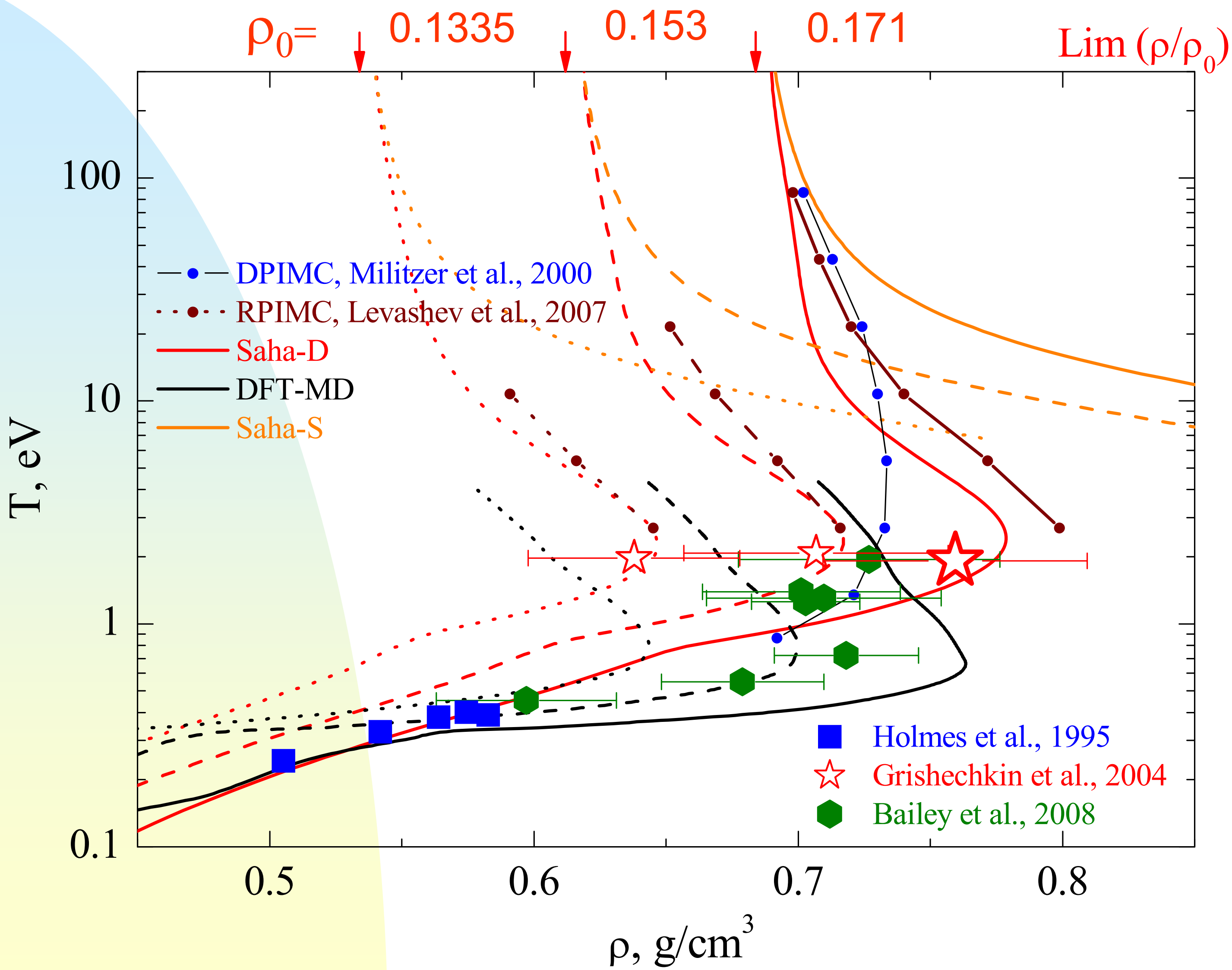

Thank you
for the attention

Liquid deuterium. Secondary shock

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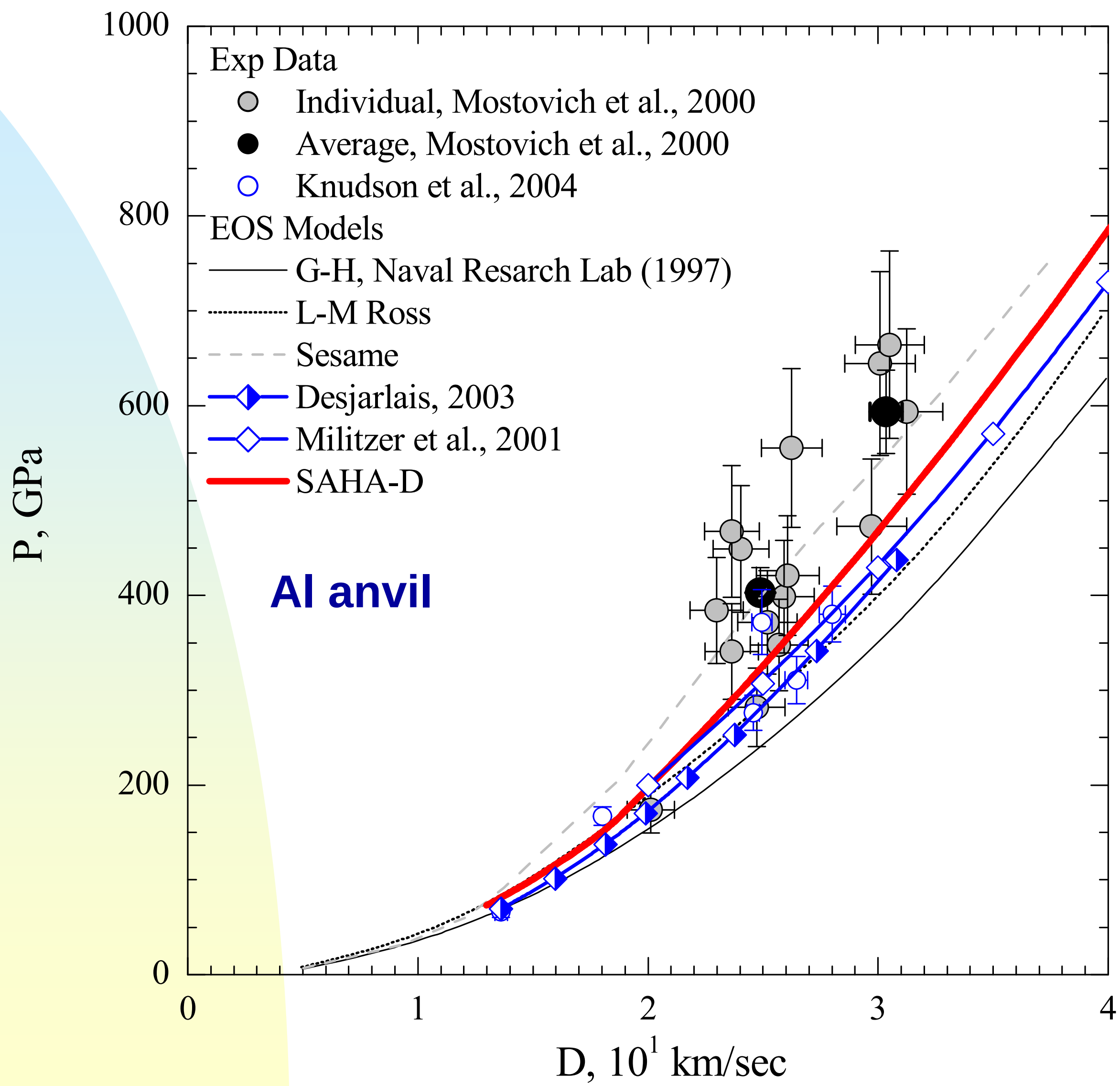
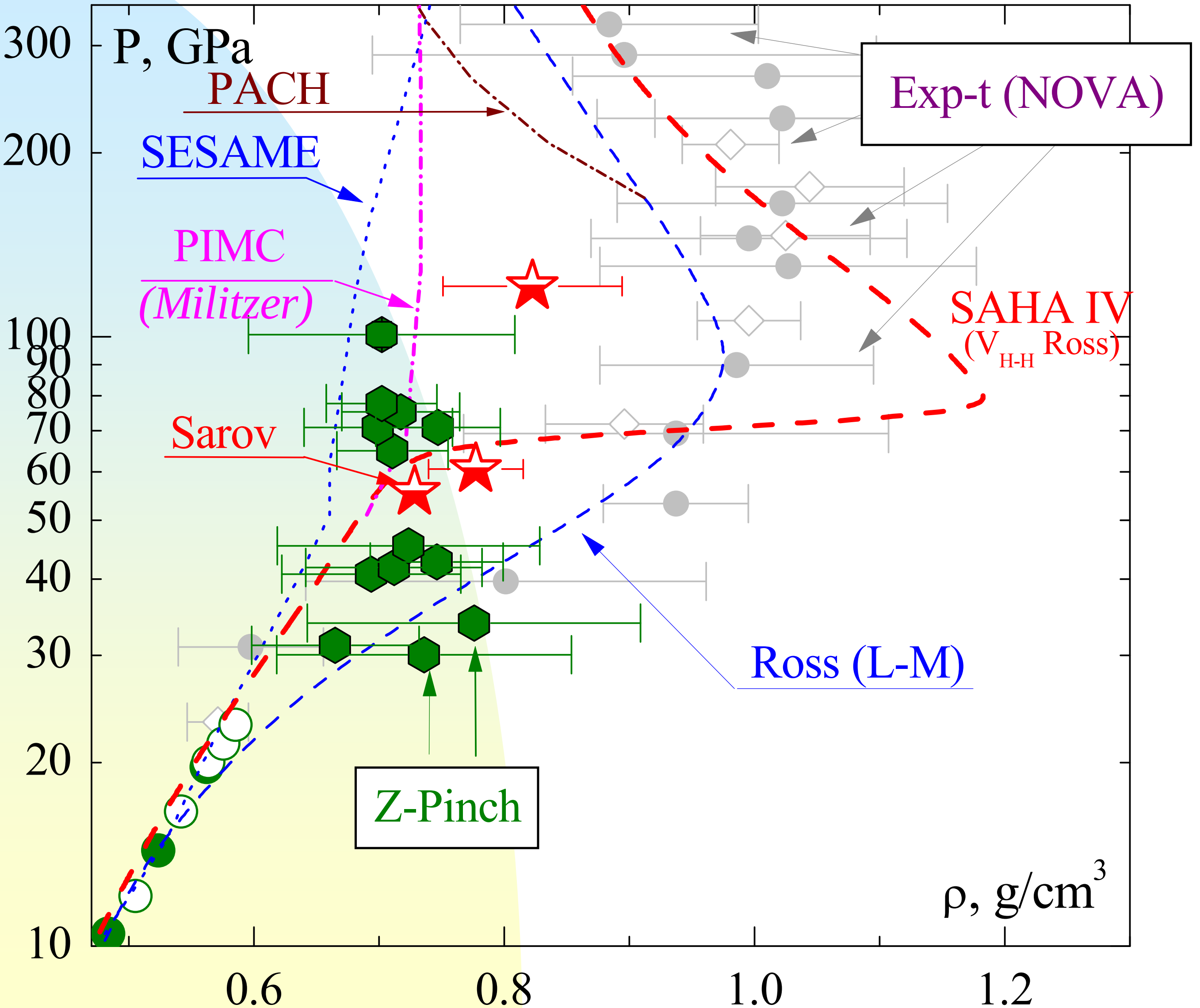


Hugoniot of Deuterium

SAHA IV - $R(D)/R(D_2) = 0.4$ - Ross, Ree&Young, *J.Chem.Phys*, **79** (1983), 1487

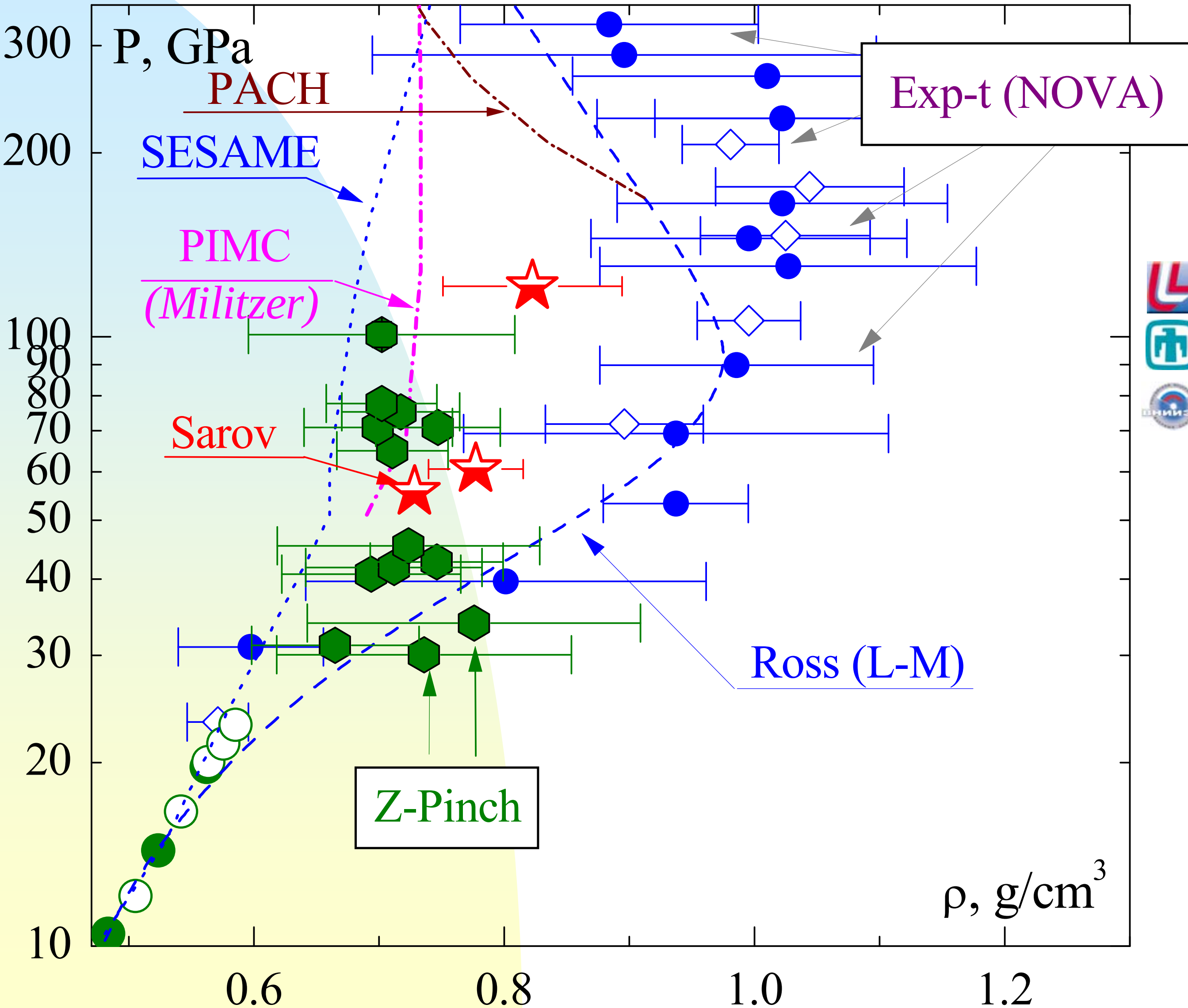


$R(D)/R(D_2) = 0.4$

Experiment:
- NOVA
- Z-Pinch (2003)
- Sarov (2002-2003)

Theory:
- SESAME Tables
- PIMC Militzer et al.
- PACH Beule et al.
- L-M Ross

Hugoniot of Deuterium



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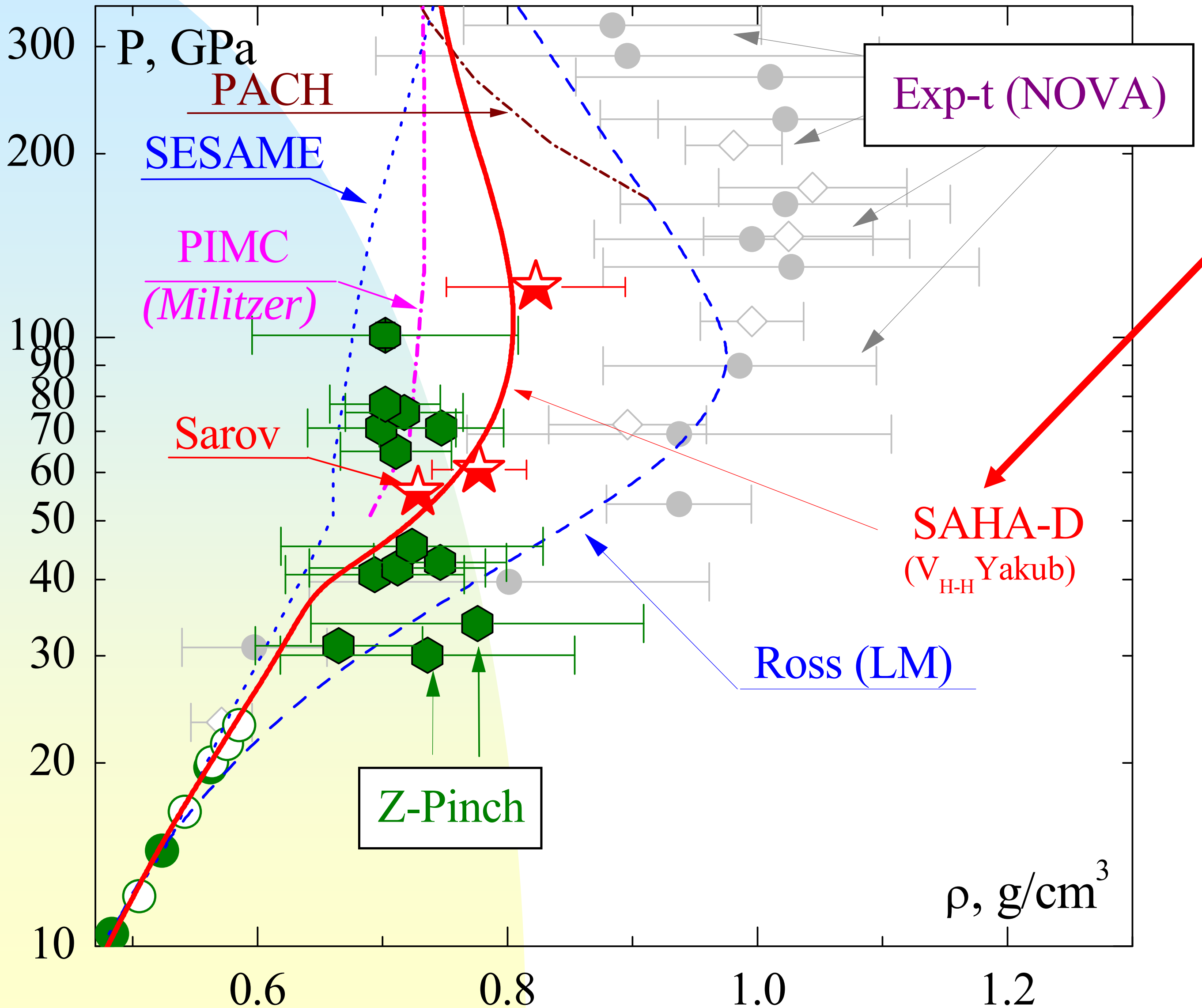
SAHA-D - $R(D)/R(D_2) = 0.8$ - E.Yakub, *High.Temp*, **28**, (1990), 664



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Theory:
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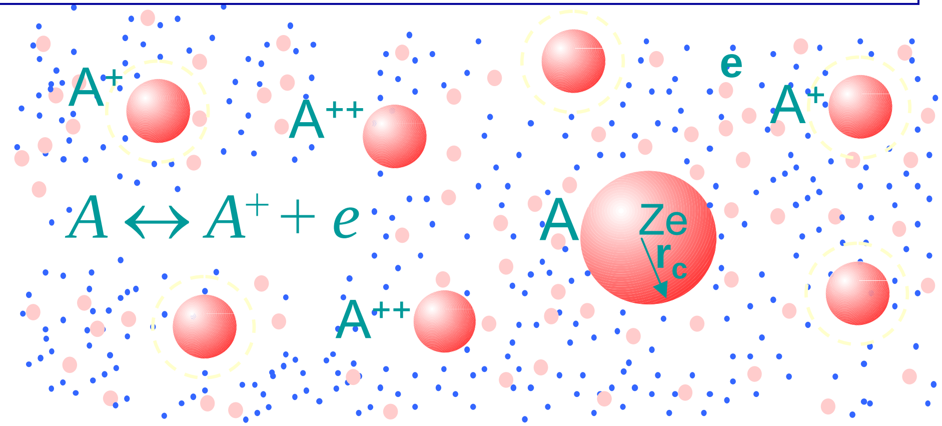
- PACH Beule et al.
- L-M Ross
- Saha-D, 2003

Chemical picture. General features of plasma models

Structure of free energy

$$F \equiv F_i^{(id)} + F_e^{(id)} + F_{ii,ie,ee,...}^{(int)}$$



Atoms, molecules, ions

$$F_i^{(id)} = \sum_{j=1}^{L} N_j k_B T \left[\ln\left(\frac{n_j \lambda_j^3}{Q_j} \right) + \frac{A_j}{k_B T} - 1 \right];$$

$$Q_j = \sum_i g_i W(\varepsilon_i, n, T) \exp\left[-\frac{\varepsilon_i}{k_B T} \right]$$

Electrons: *(arbitrary degeneracy)*

$$F_e^{(id)} = \frac{4Vk_B T}{\pi^{1/2}\lambda_e^3} \left[\alpha_e I_{1/2}(\alpha_e) - \frac{2}{3} I_{3/2}(\alpha_e) \right]$$

$$\alpha_e = \mu_e / k_B T; \quad \frac{n_e \lambda_e^3}{2} = \frac{\sqrt{\pi}}{2} I_{1/2}(\alpha_e)$$

Nonideality effects : $F_{ii,ie,ee,...}^{(int)}$

Coulomb interaction: pseudopotential model, modified Debye approximations, ...

Strong short range repulsion between all species: atoms and molecules - spheres of nonzero radius...

Neutral-neutral short range attraction

Partition functions: $Q_j = Q_j(\varepsilon_i, \{n_j\}, T)$

Dependence of partition functions on density and temperature

Non-empirical atom–atom approximation

E.Yakub, *High.Temp*, **28**, (1990), 664

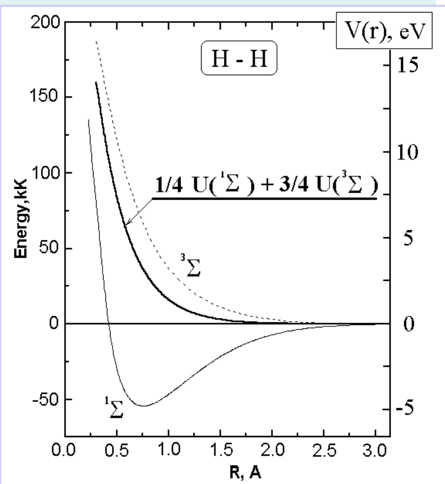
Effective atomic diameters and inter-atomic distances in H_2 molecule

T, K	1000	2000	4000	6000	8000	10000
σ_H	*1.93*	*1.78*	*1.62*	*1.52*	*1.45*	*1.40*
$L_{H–H}$	*0.76*	*0.77*	*0.81*	*0.86*	*0.91*	*0.95*

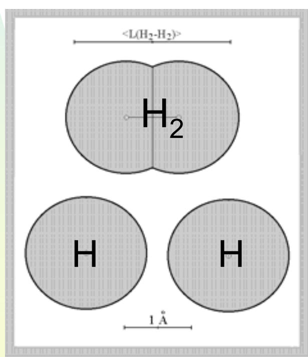
$$\Phi_{H\text{-}H}(r) = (1/4)U(^1\Sigma|r) + (3/4)U(^3\Sigma|r)$$

SAHA-D

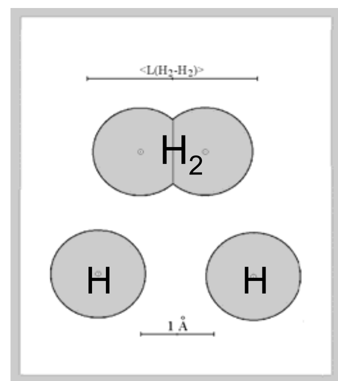
$R(D)/R(D_2) = 0.8$



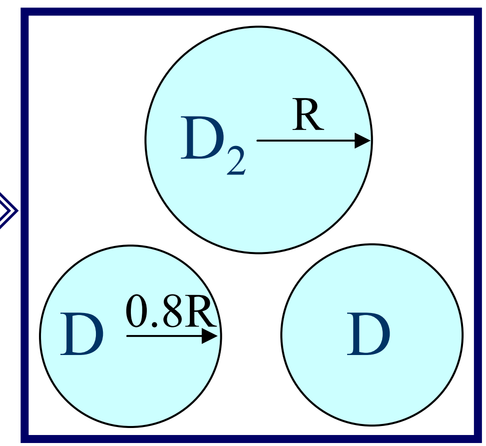
Atom-atom potential
for “free” hydrogen atoms



T = 2000 K



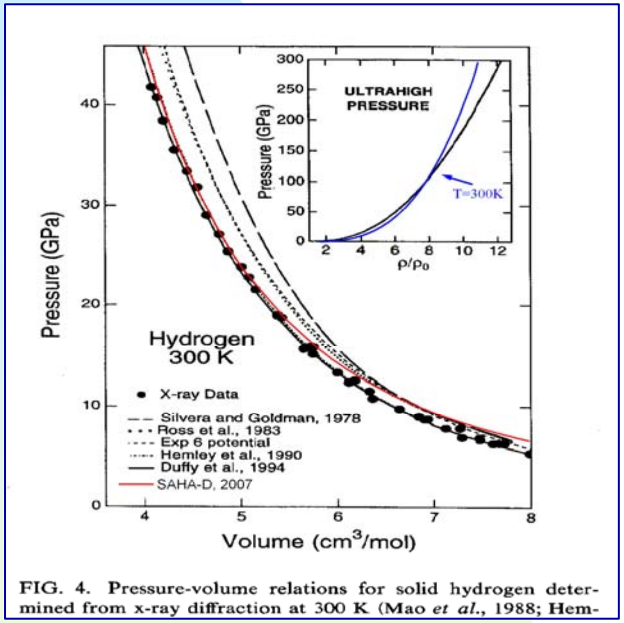
T=10000 K

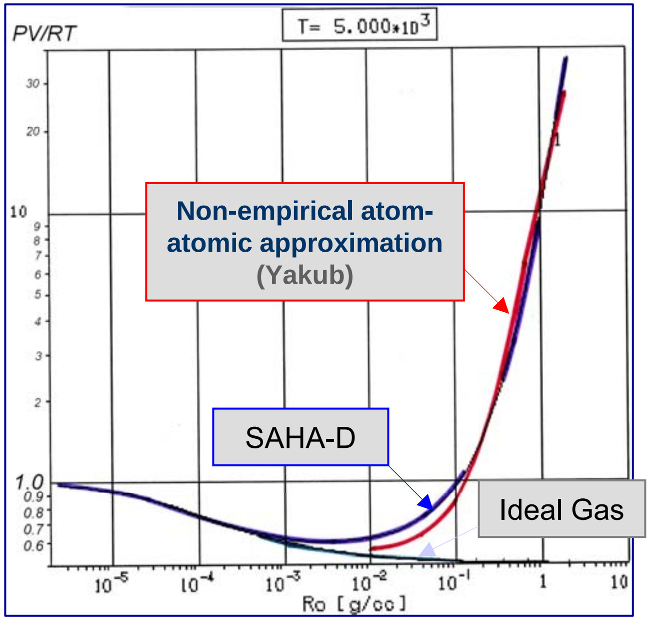


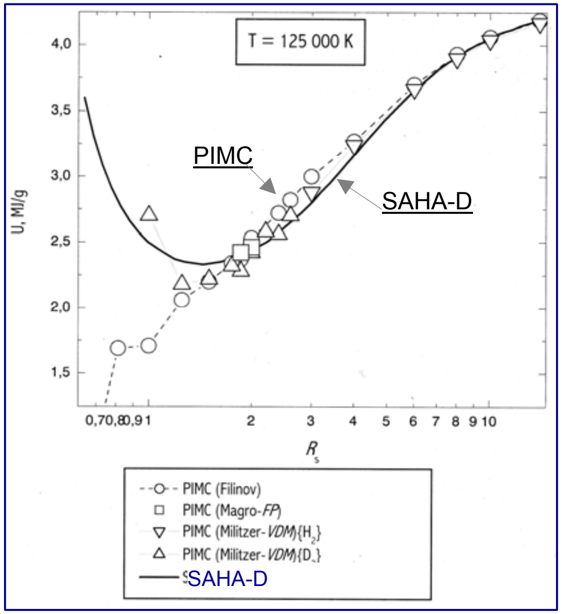
It is equivalent to
approximately
equal “volumes” in reaction:
$H_2 \leftrightarrow 2H$ ($D_2 \leftrightarrow 2D$)

Validation of SAHA-D model

Soft-sphere approximation for EOS of Hydrogen







Isotherm T = 300 K

Comparison with experiment

Mao H.K., Hemley R.J. *Rev. Mod. Phys*. 66 671 (1994)

Isotherm T = 5’000 K

Comparison with *non-empirical* atom-atomic approximation

AAP -Yakub E.S. *Physica* B 265 31 (1999)

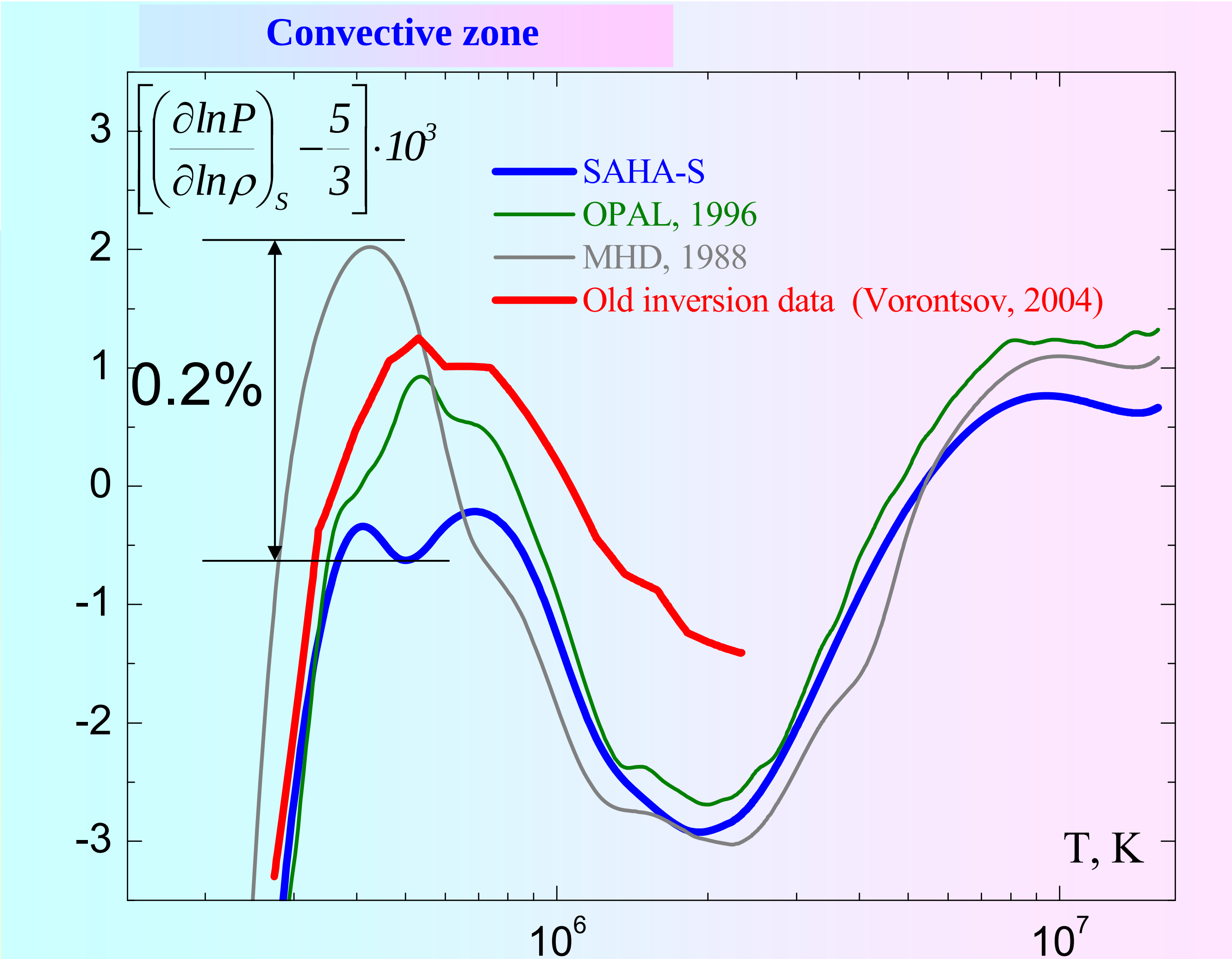
Isotherm T = 125’000 K

Comparison with *ab-initio* approach

Ab-initio approach. *Phys. Rev.Lett* 85 1890 (2000)

SAHA-S

Models and old inversion data

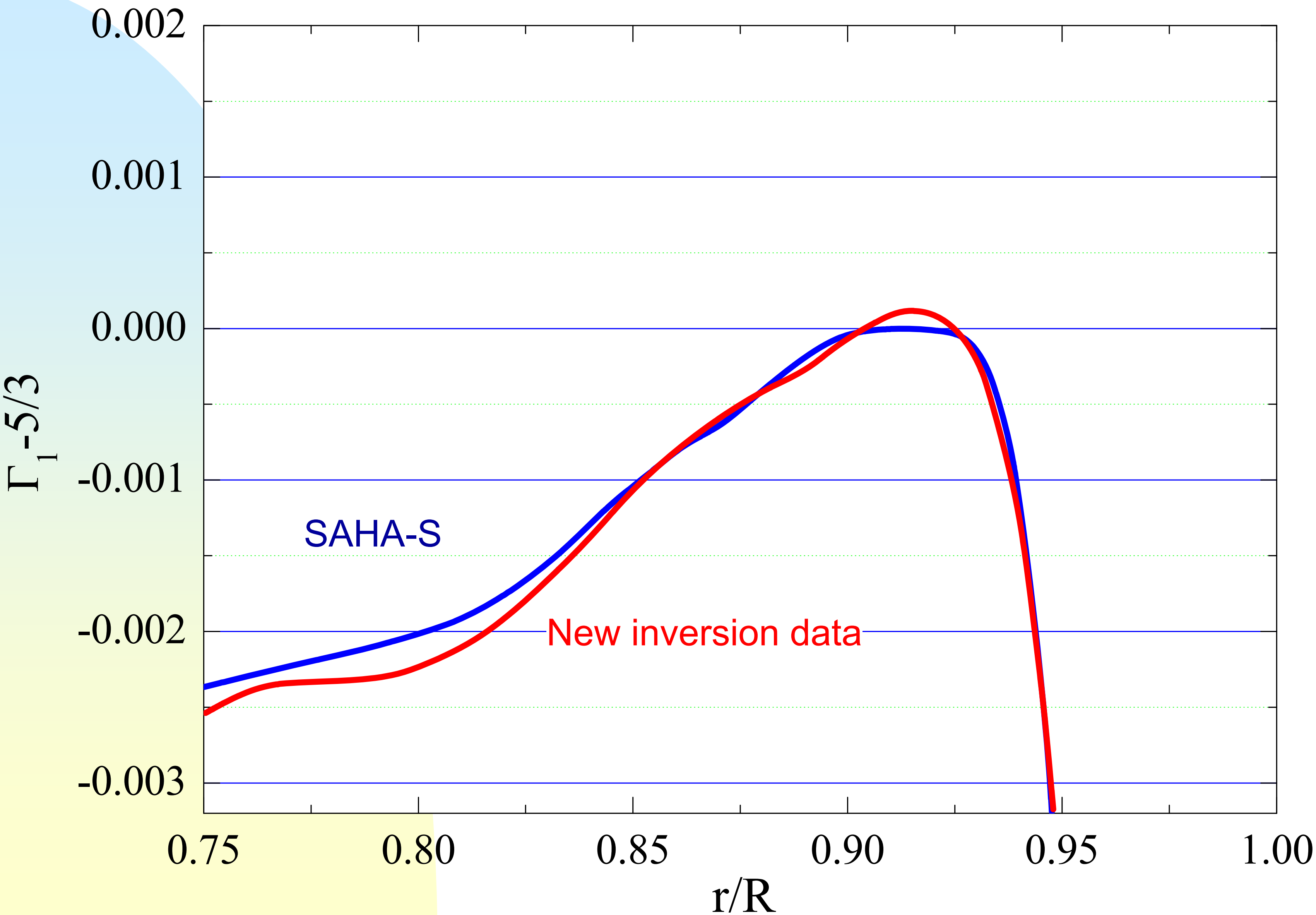


SAHA-S – asympthotically exact model for thermodynamics of solar plasma

V.Gryaznov, S.Ayukov, V.Baturin, I.Iosilevskiy, A.Starostin and V.Fortov *J. Phys. A* **39** 4459 (2006)

Helioseismology

SAHA-S and **NEW** inversion data (December 2008).



Summary

- Saha-D model has been applied to calculation of equation of state of warm dense deuterium.
- Comparison of Saha-D calculation results with single and double shock experimental data demonstrates good agreement.
- At high temperature limit Saha-D model coincides with asympthotically exact theoretical approximation (SAHA-S)

Outlook

- Saha-D has to be applied to experimental data of strong isentropic compression of deuterium
- Saha-D has to be applied to shock compression data of helium and nitrogen of megabar pressure range

Thank you for the attention!