Уравнение состояния ударно-сжатого дейтерия

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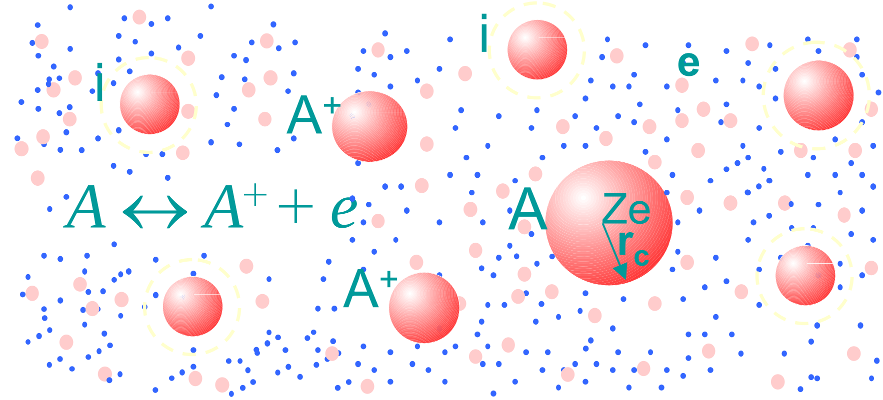
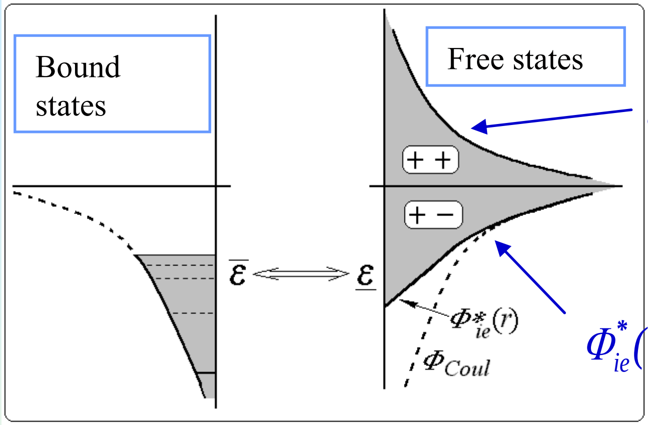
Основные характеристики

- Вещество рассматривается как сильно взаимодействующая многокомпонентная частично ионизованная смесь атомов, молекул, ионов и электронов
- Кулоновское взаимодействие заряженных частиц: модифицированная псевдопотенциальная модель (И.Иосилевский)
- Интенсивное короткодействующее отталкивание: модифицированная модель «мягких сфер (D.Young)
- Частичное вырождение электронов

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

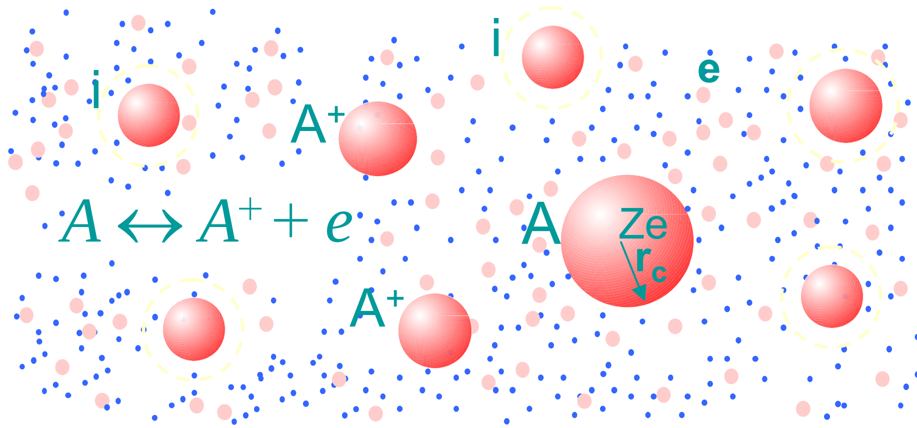
$$\Delta P^{(Coul)}$$

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

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

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

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

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

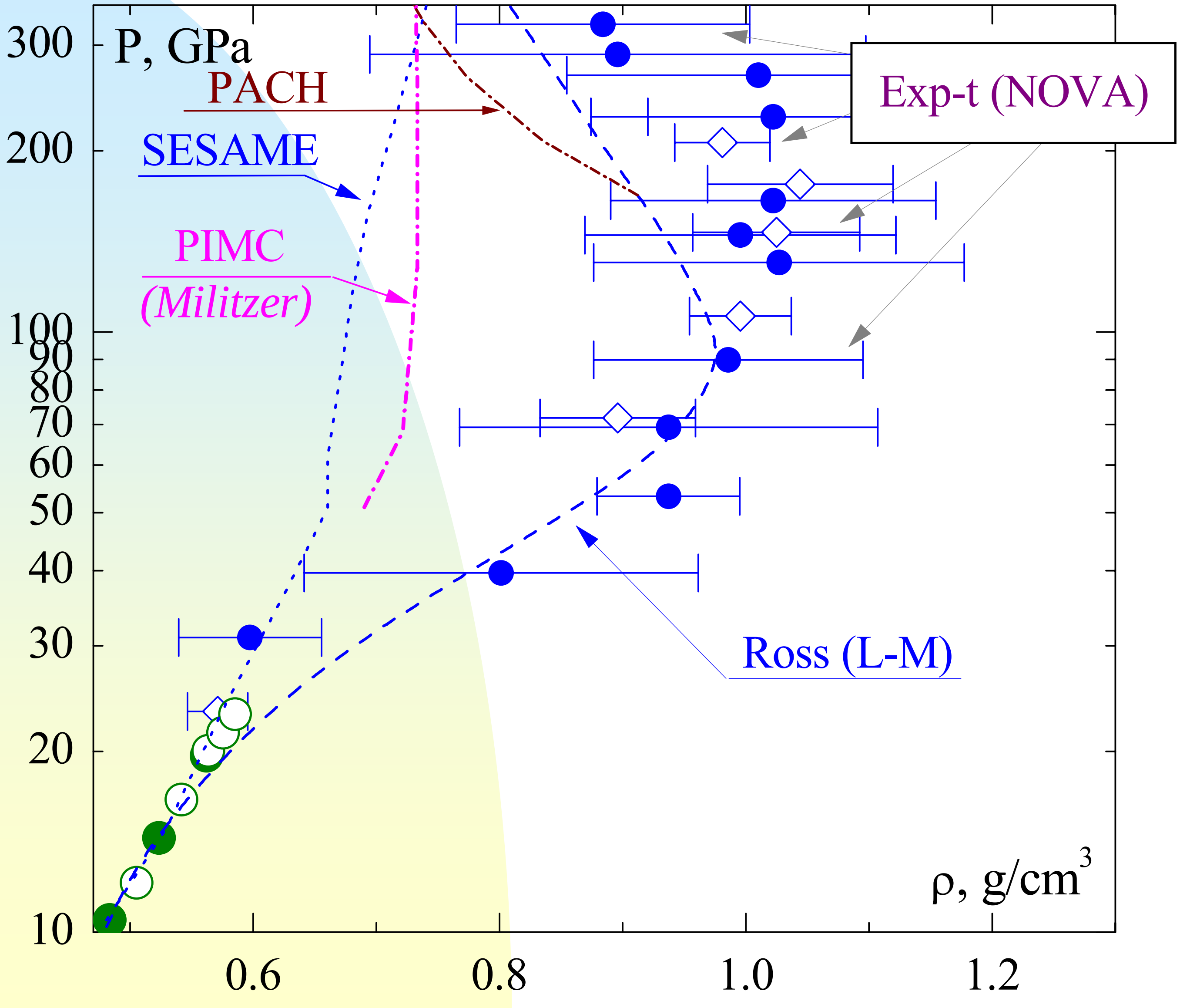
$$y = \frac{3Y\sqrt{2}}{\pi}; \quad Y = \frac{4\pi r_c^3}{3} = \frac{\pi \sigma_c^3}{6}$$

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**

Hugoniot of Deuterium

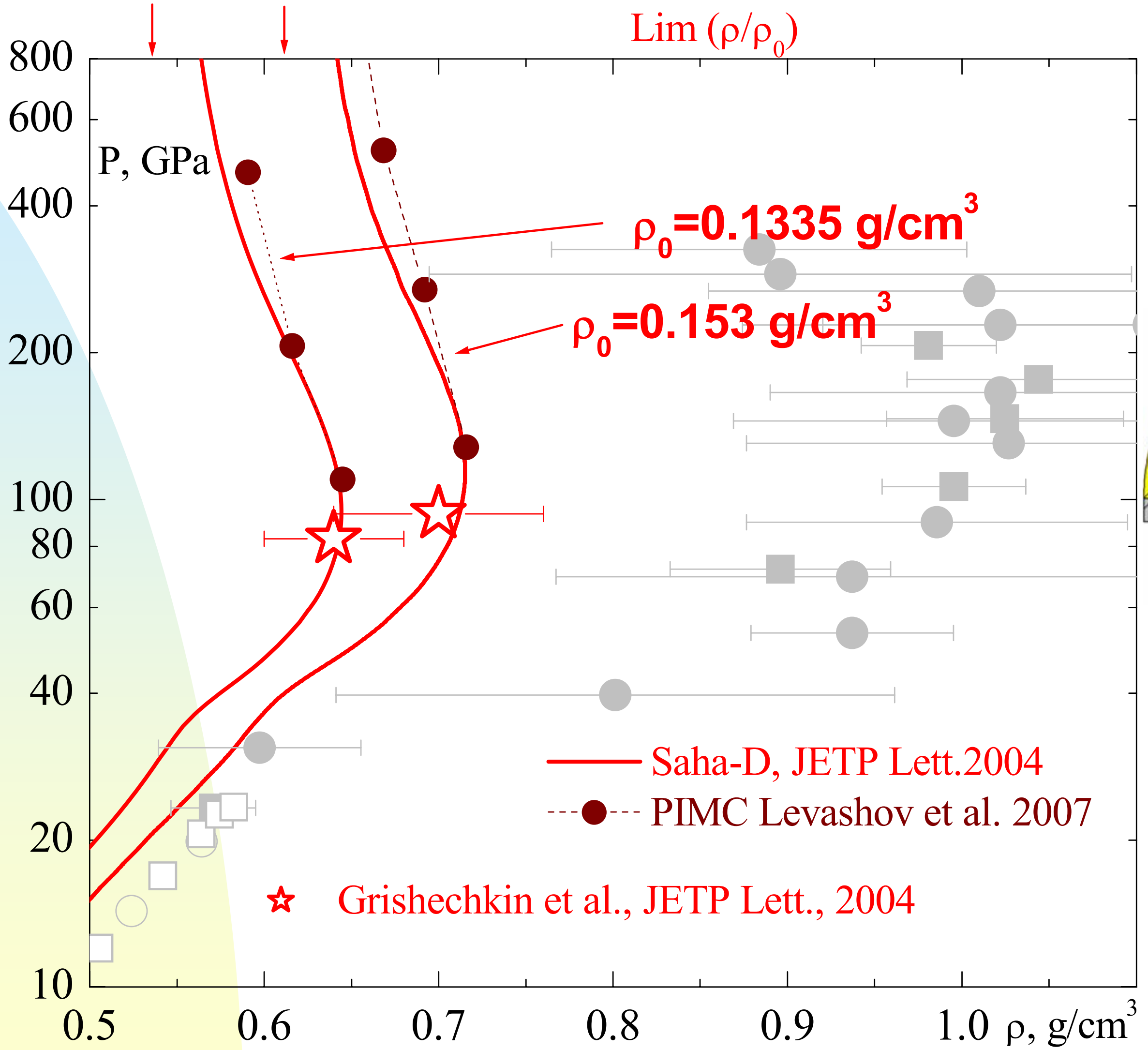


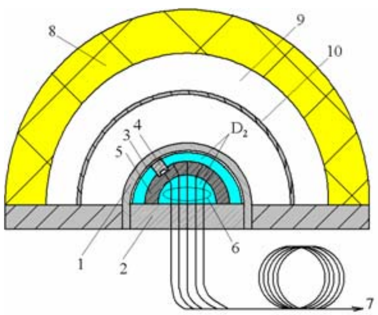
Experiment:
- NOVA

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

Hugoniots of precompressed deuterium

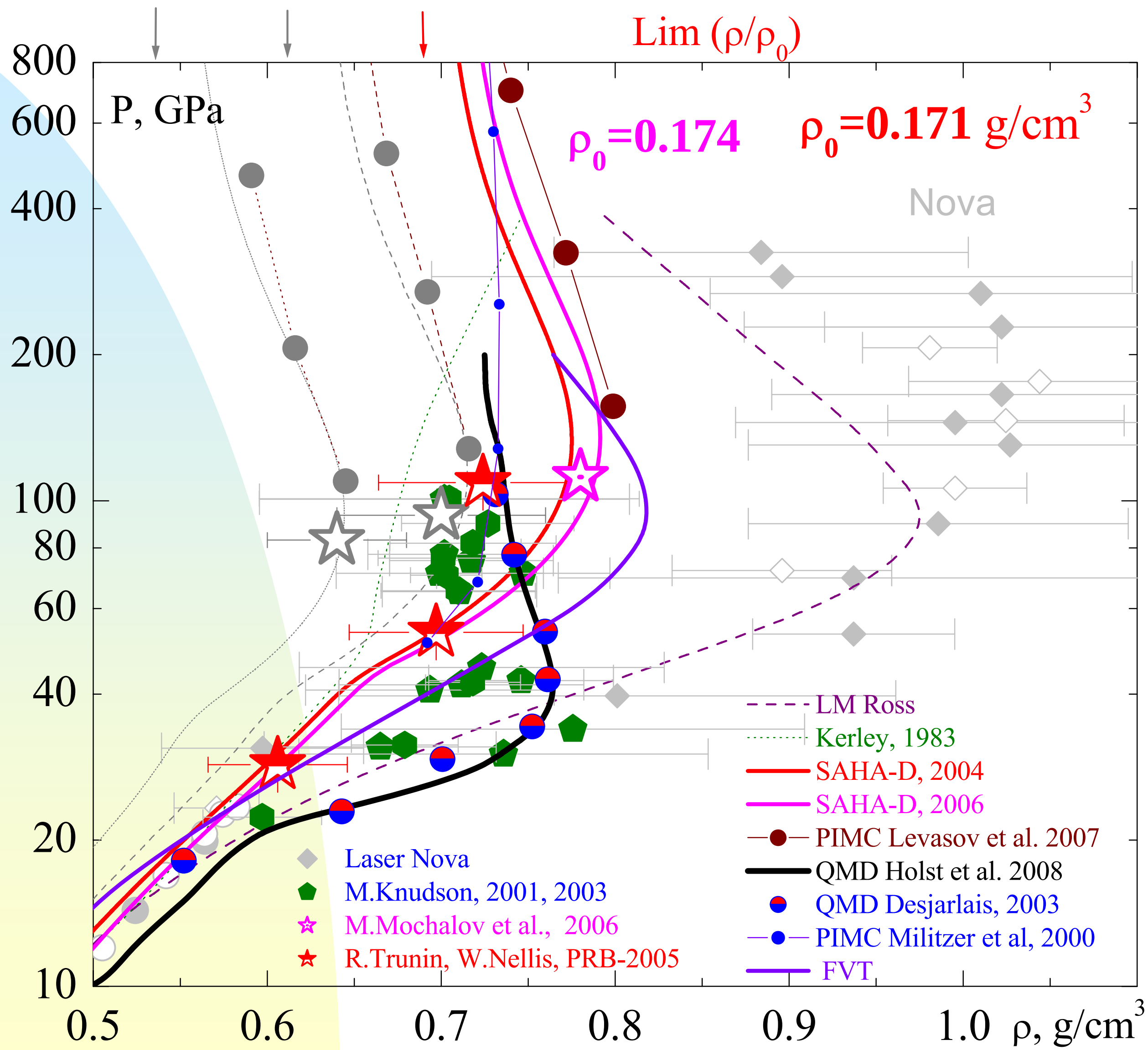
Experimental data and model calculations

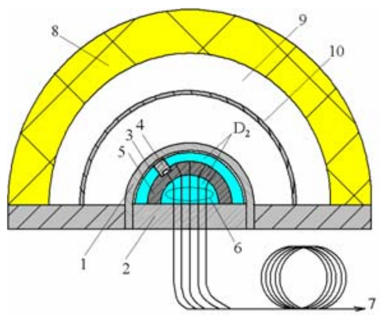




Hugoniots of liquid deuterium

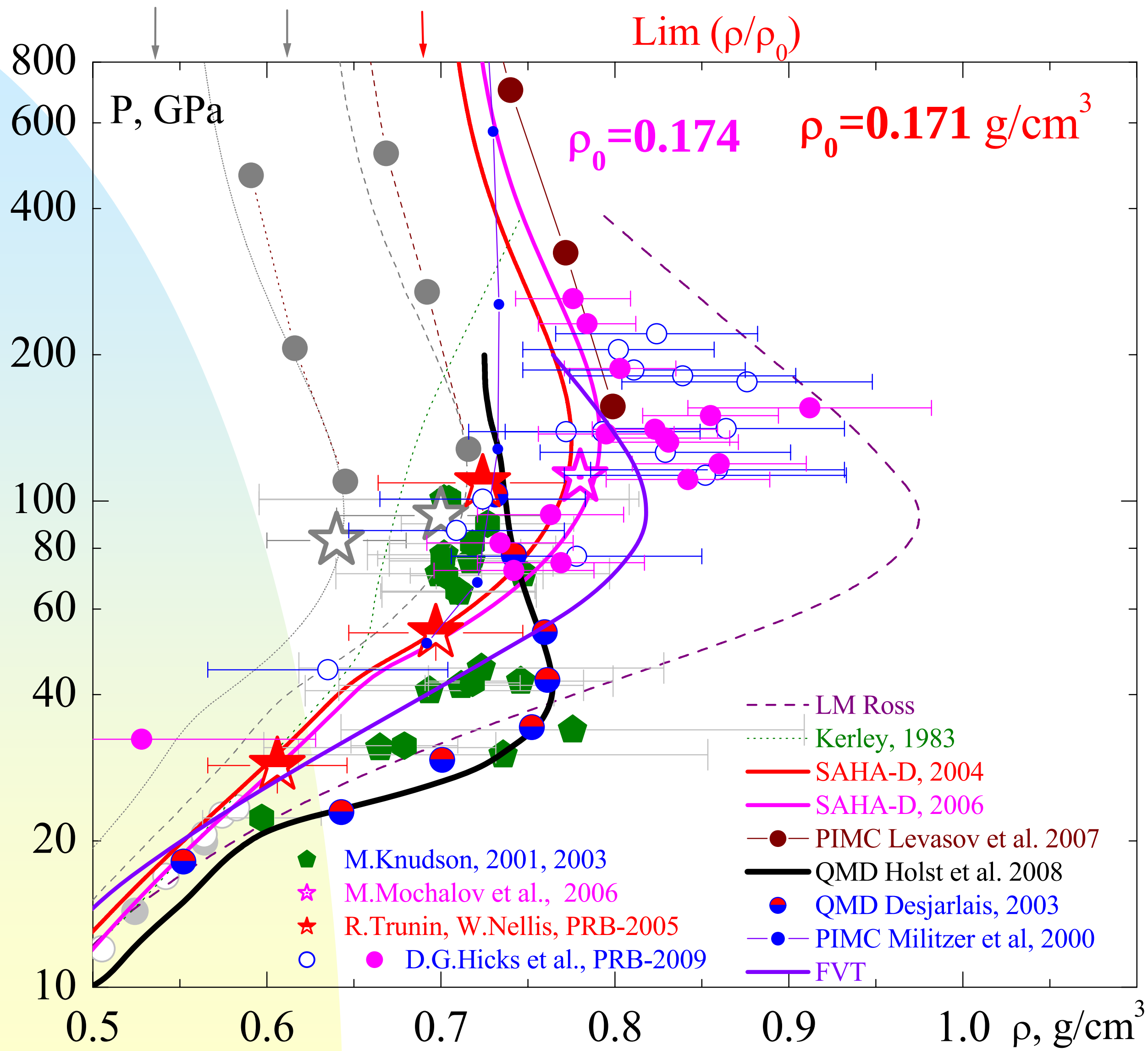
Experimental data and model calculations





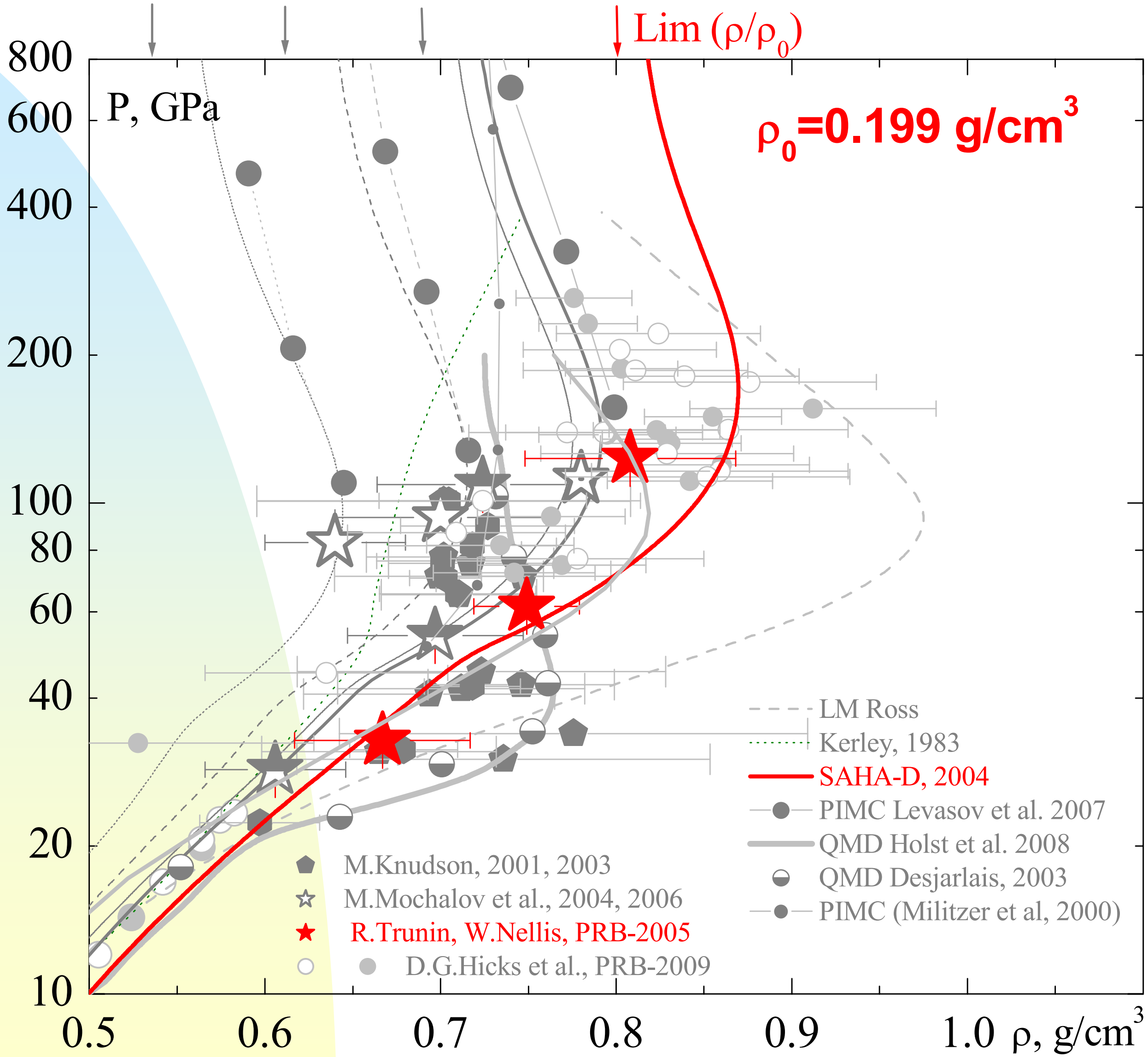
Hugoniots of fluid deuterium

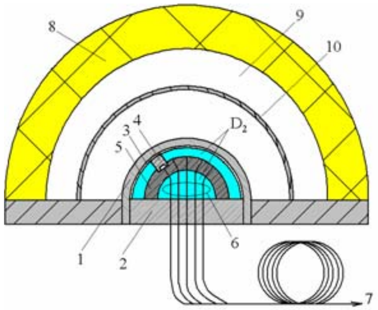
New experimental data and model calculations



Hugoniots of solid deuterium

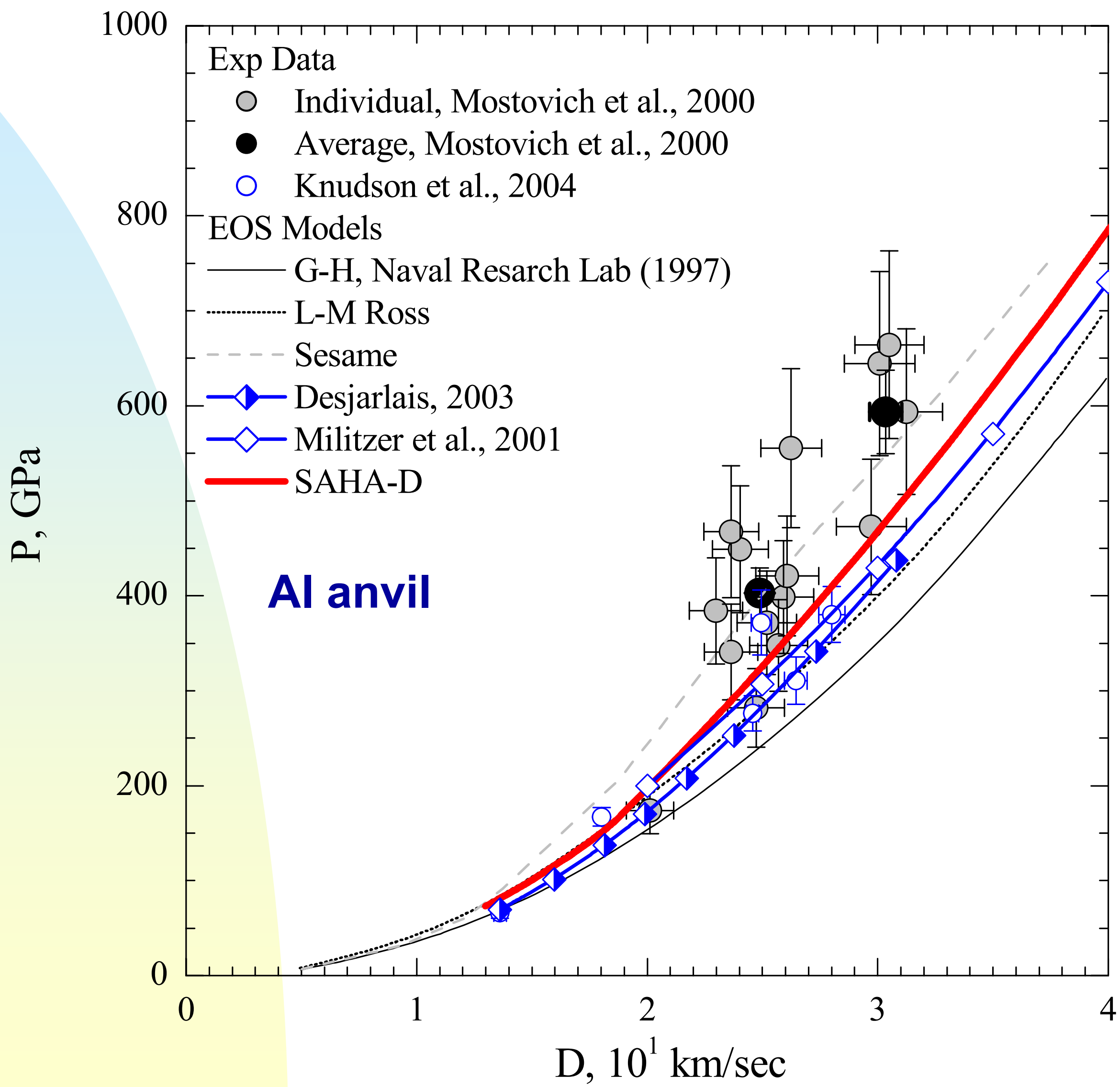
Experimental data and model calculations





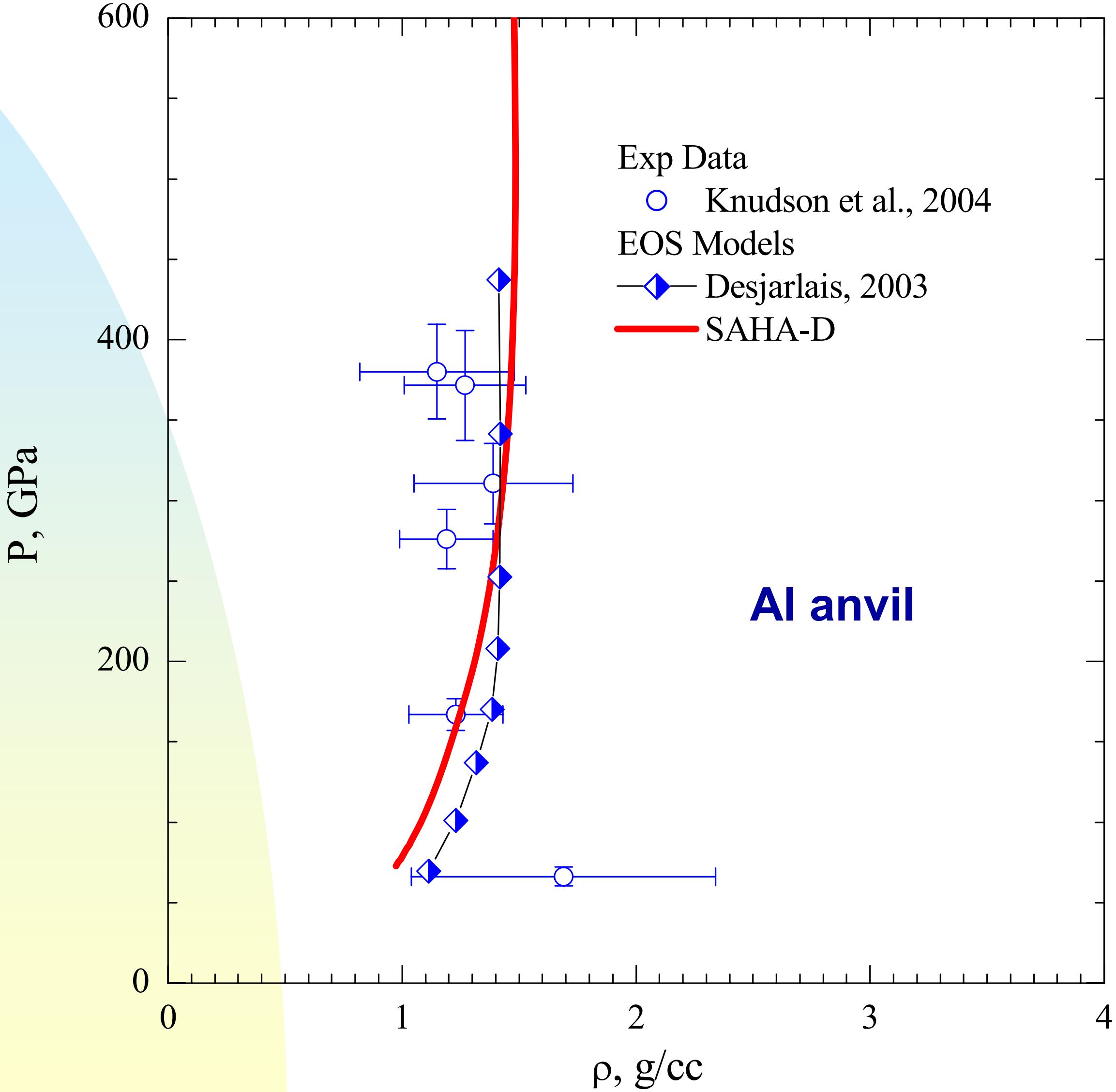
Liquid deuterium. Secondary shock

Experimental data and model calculations

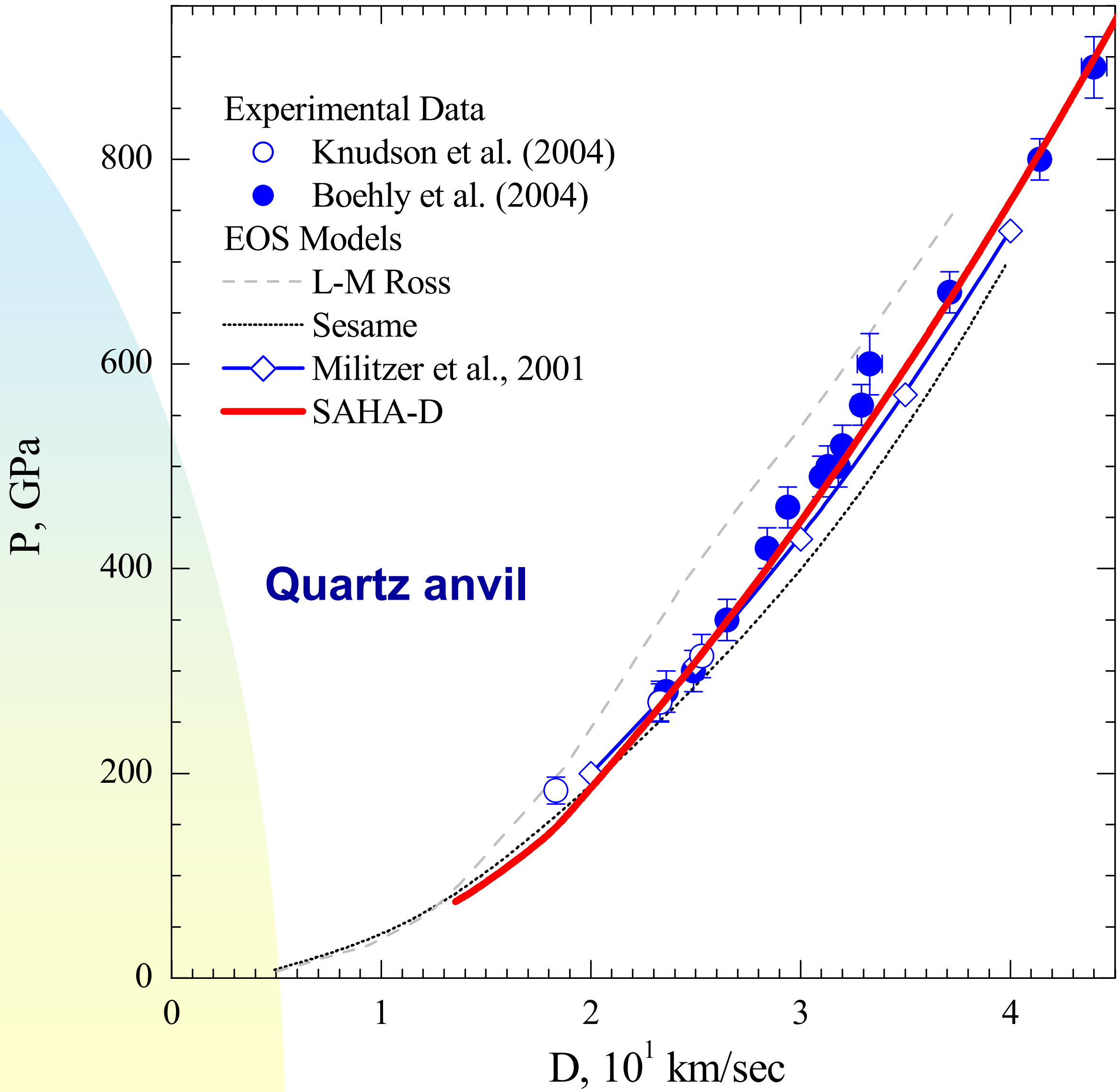


Liquid deuterium. Secondary shock

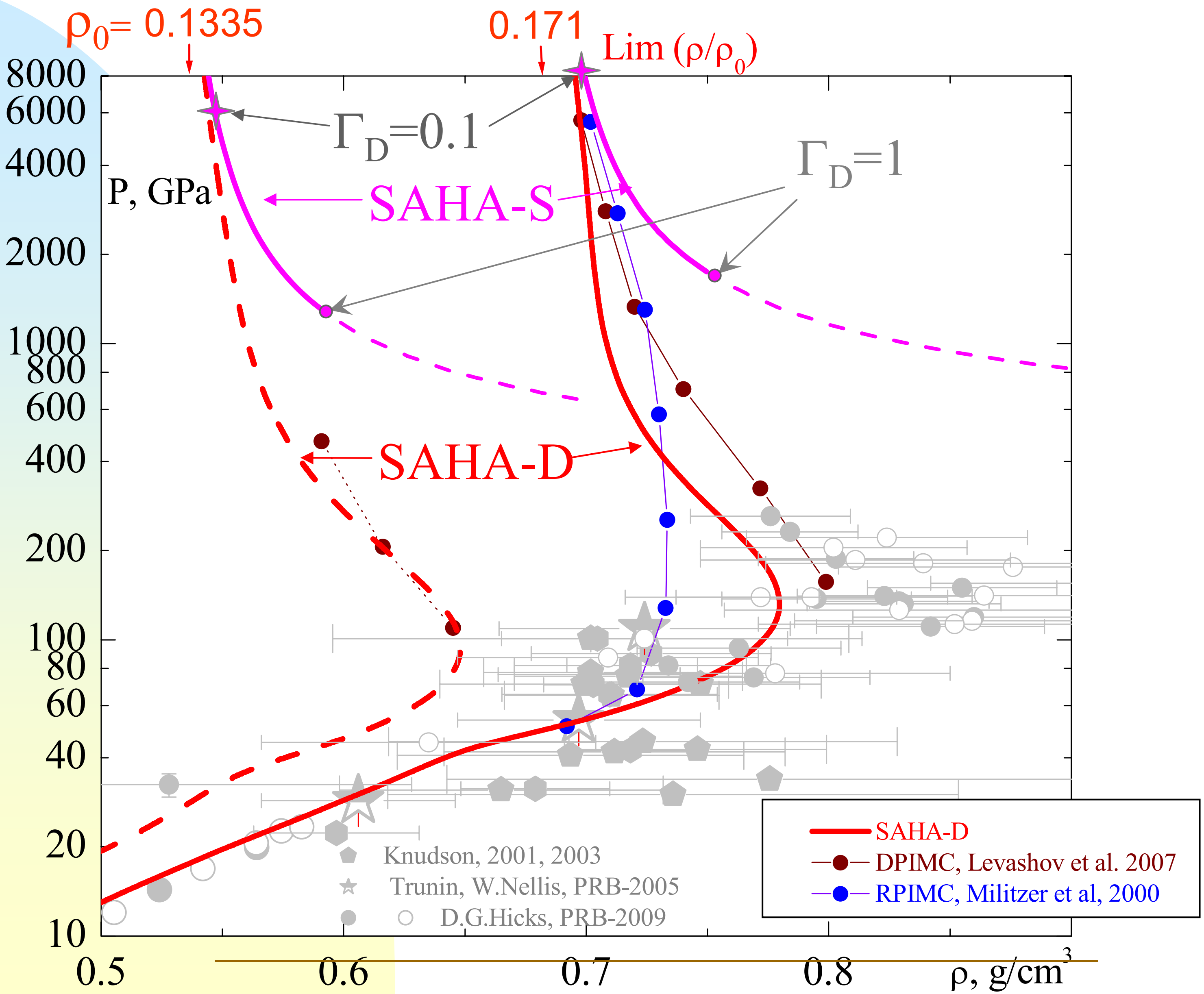
Experimental data and model calculations



Liquid deuterium. Secondary shock
Experimental data and model calculations

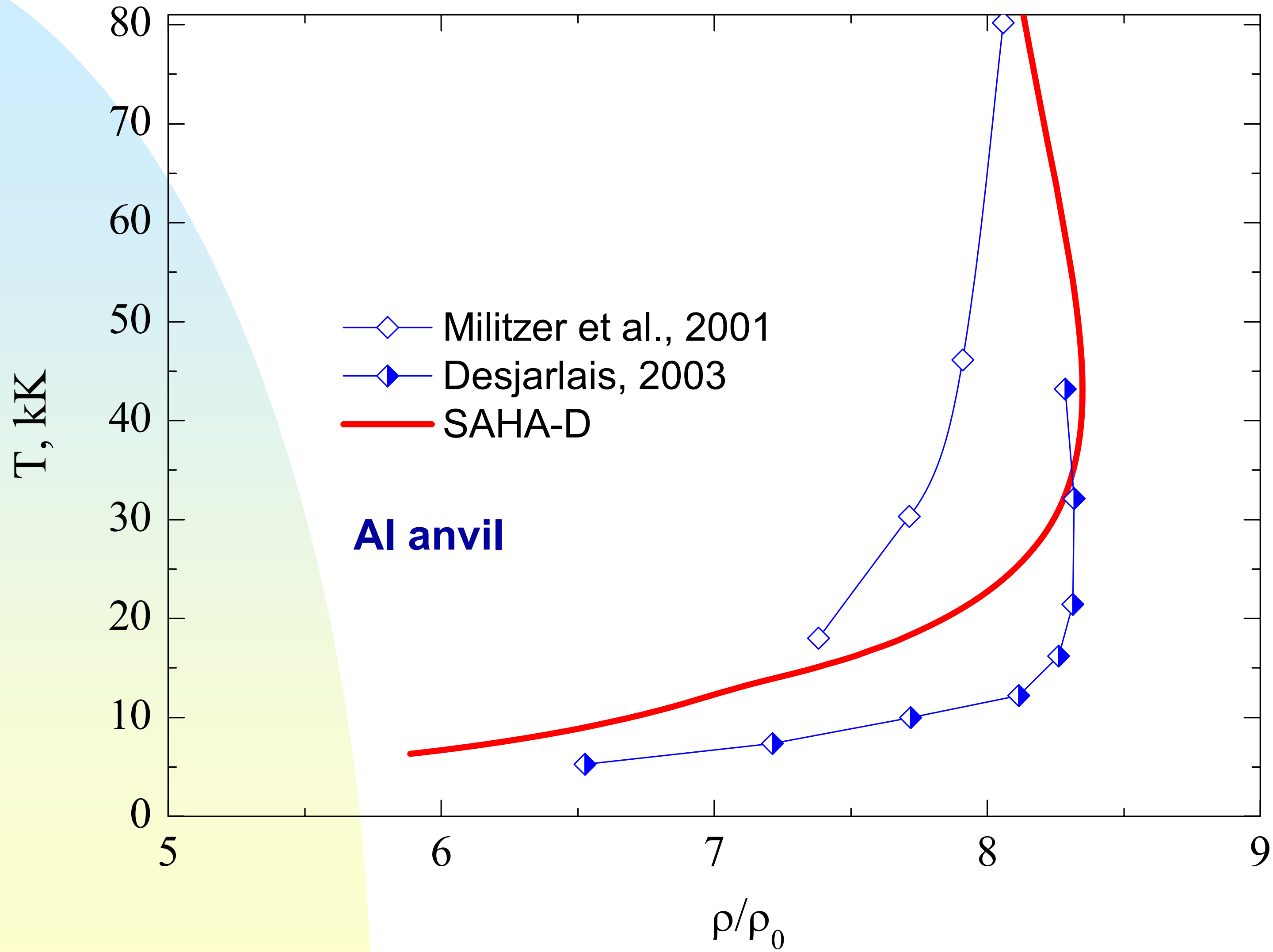


Validation of high-temperature asympthotics



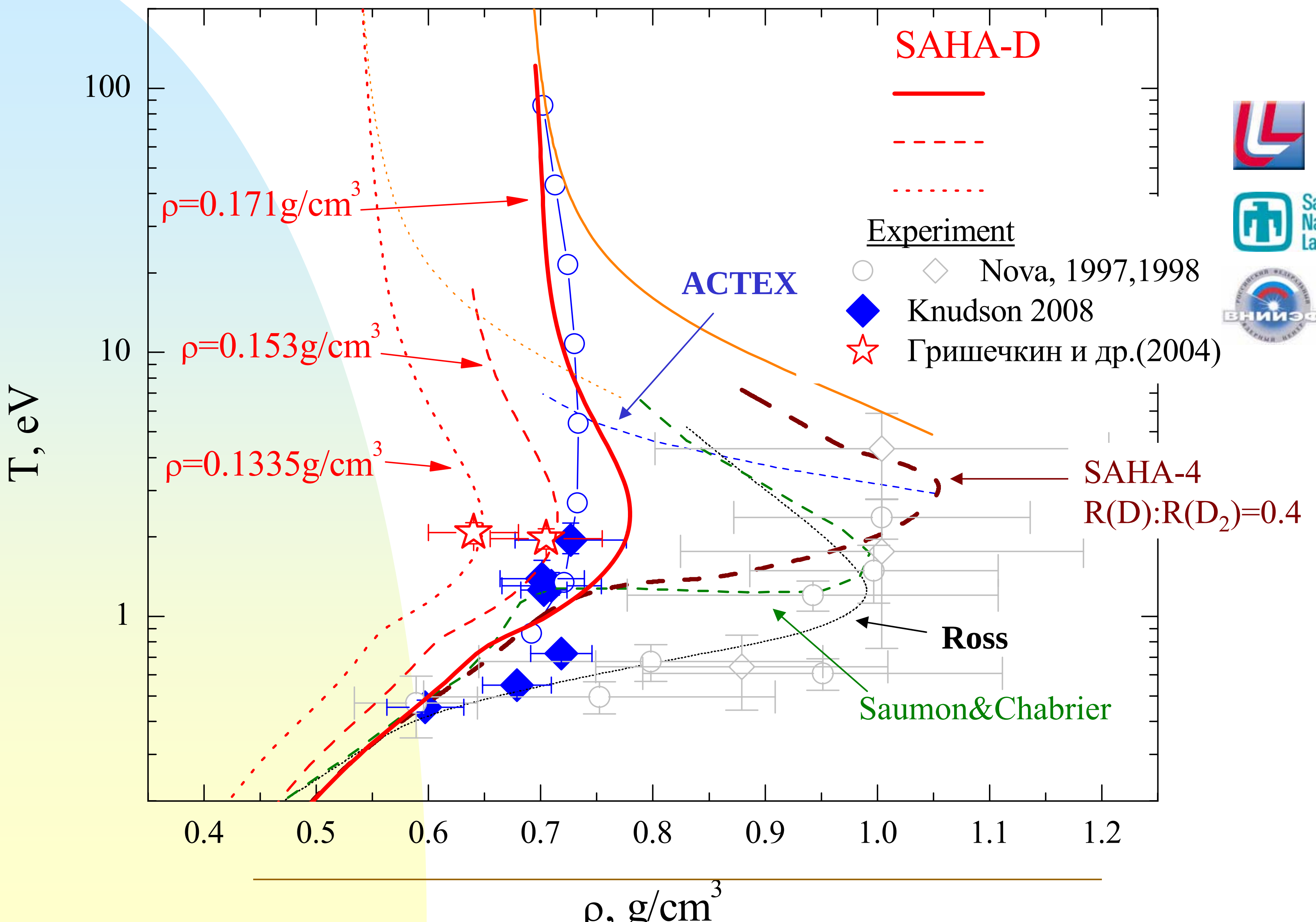
Liquid deuterium. Secondary shock

Model calculations



Hugoniots of fluid deuterium

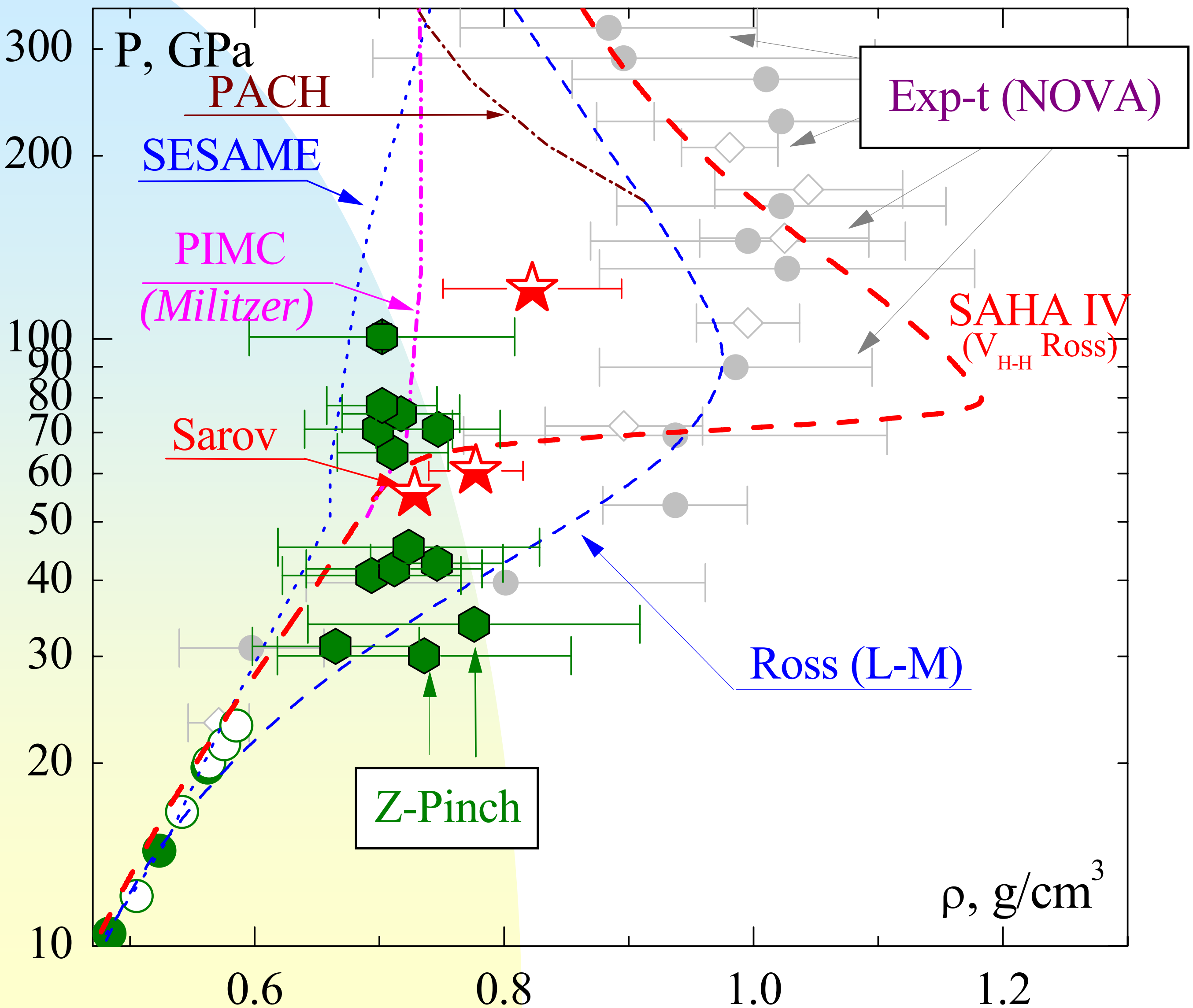
New experimental data and model calculations



Спасибо!

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:
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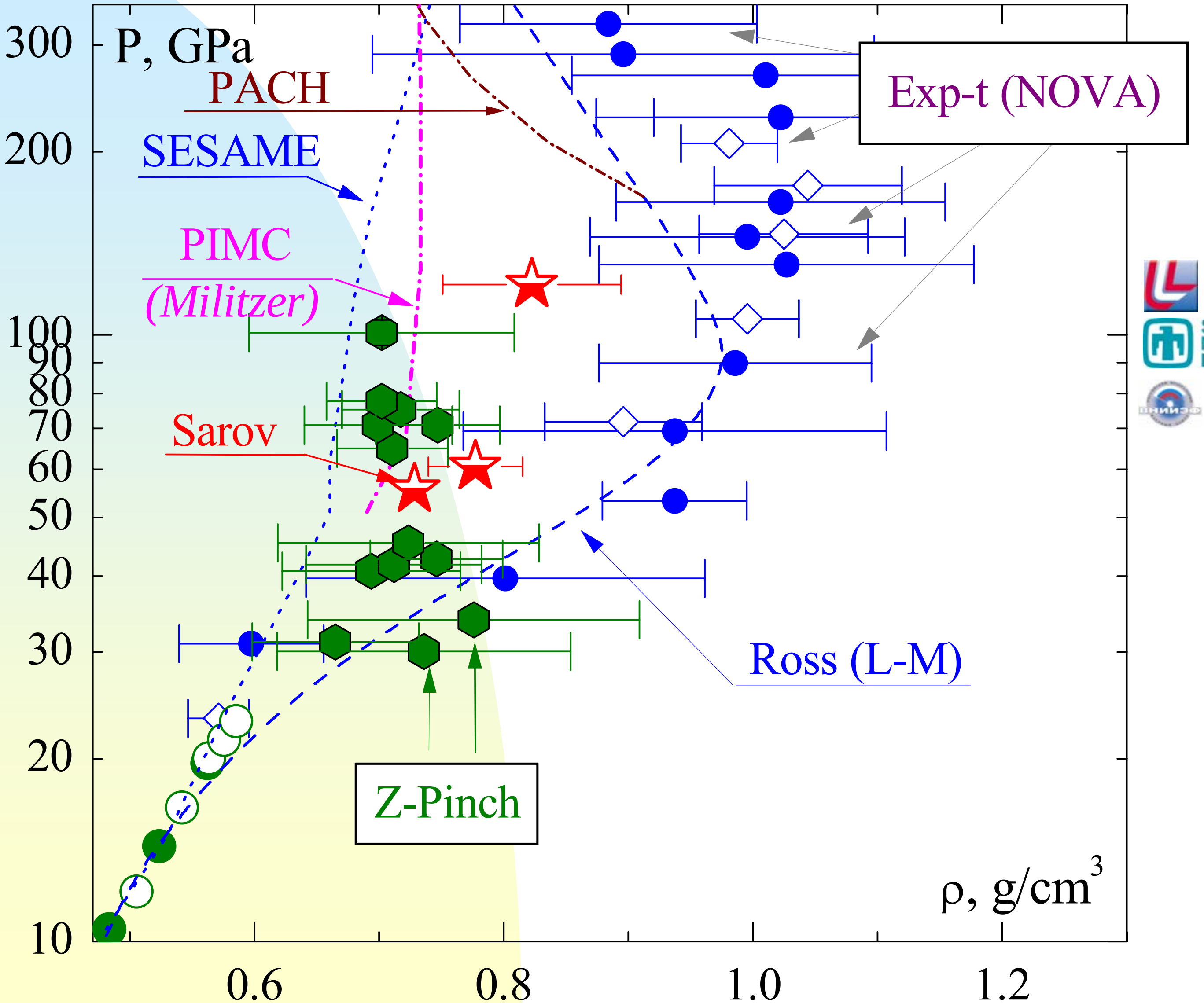
Hugoniot of Deuterium



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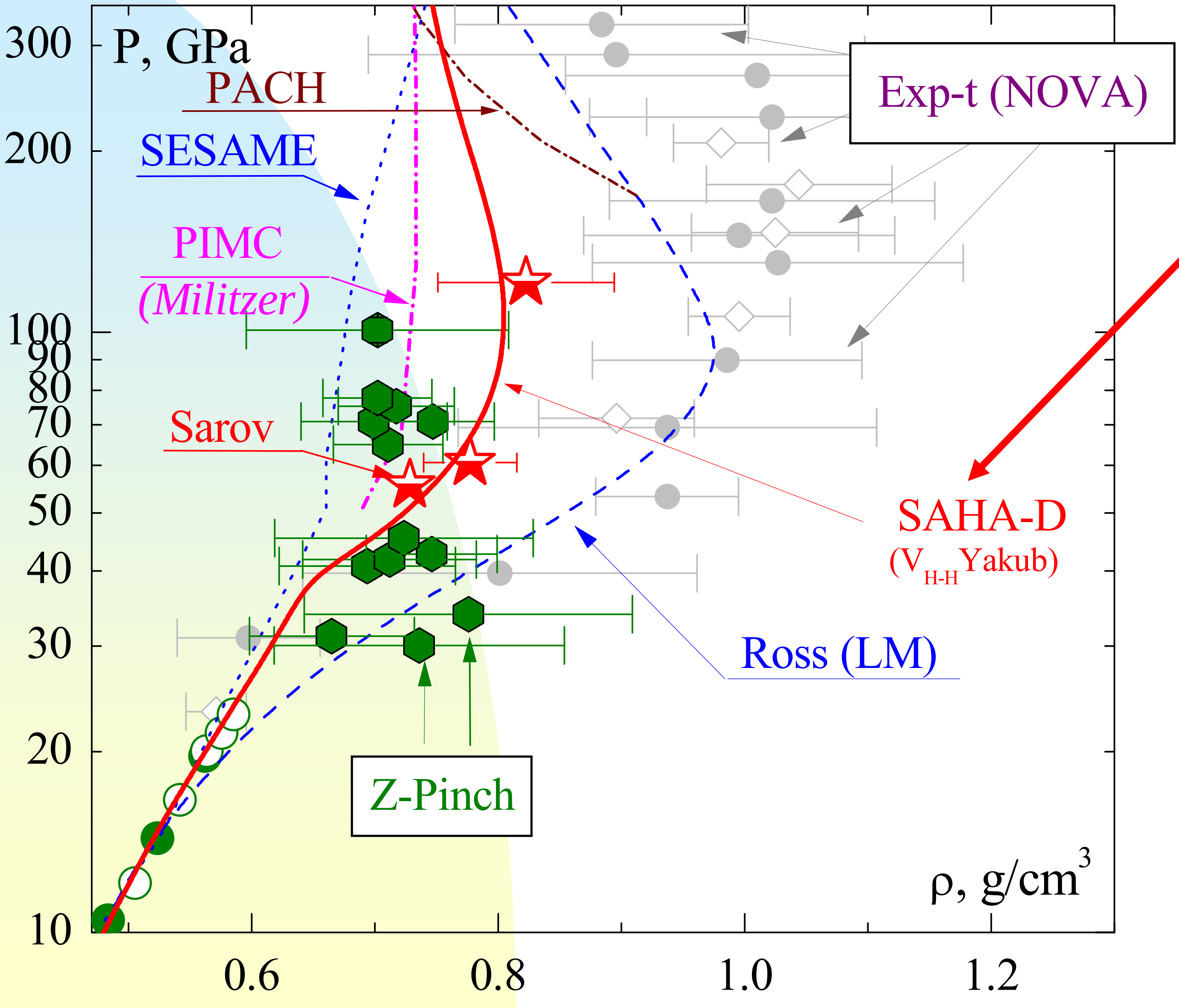
Hugoniot of Deuterium

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



R(D)/R(D_2) = 0.8

Experiment:
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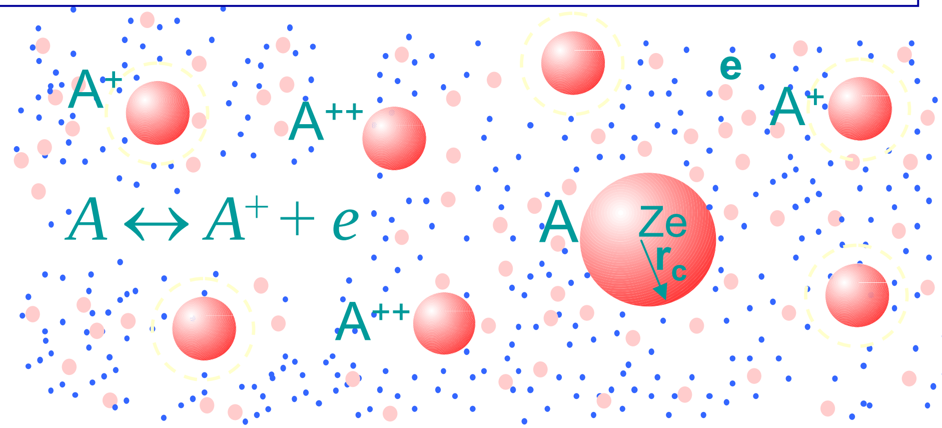
Theory:
- SESAME Tables
- PIMC Militzer et al
- PACH Beule et al.
- L-M Ross
- Saha-D, 2003

Chemical picture. General features of plasma models



Structure of free energy

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

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 : $F_{ii,ie,ee,\ldots}^{(int)}$

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

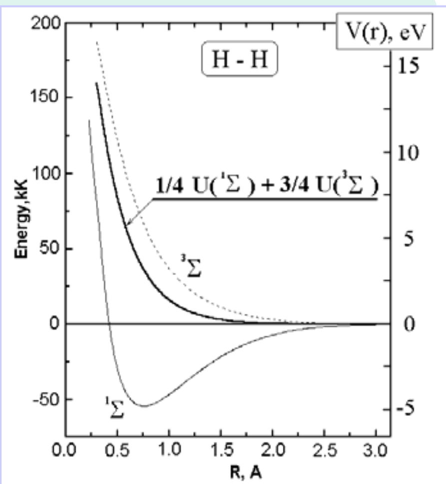
Effective atomic diameters and inter-atomic distances in H_2 molecule

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*

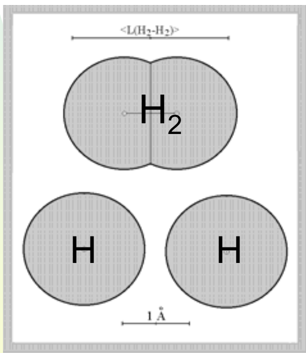
$$\Phi_{H\text{-}H}(r) = (1/4)U(^1\Sigma|r) + (3/4)U(^3\Sigma|r)$$

SAHA-D

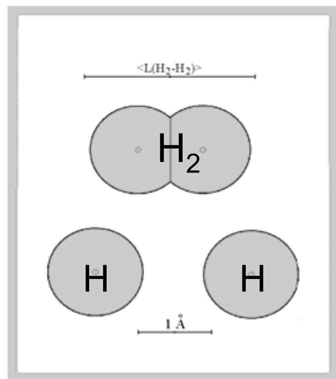
$R(D)/R(D_2) = 0.8$



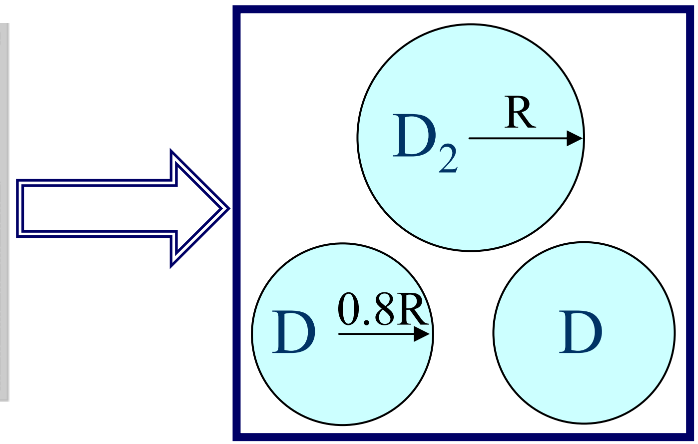
Atom-atom potential
for “free” hydrogen atoms



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

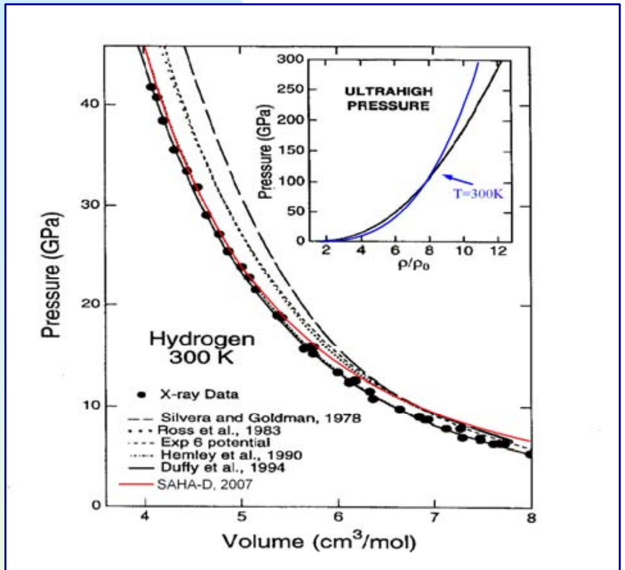
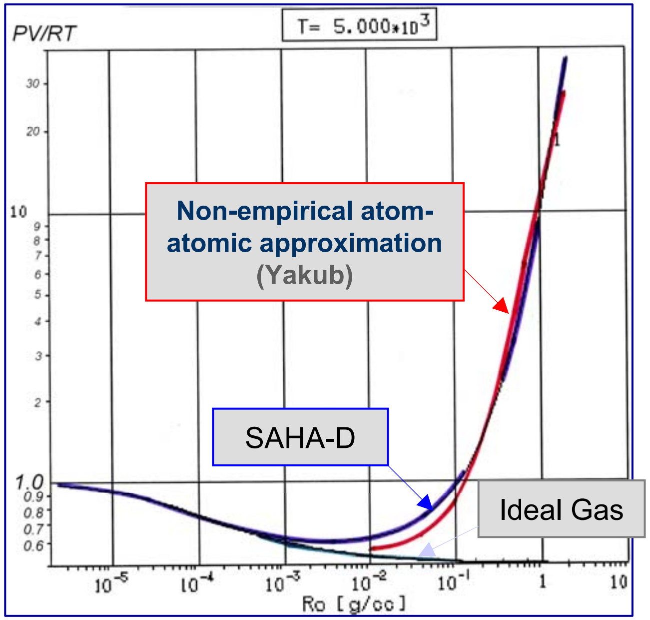
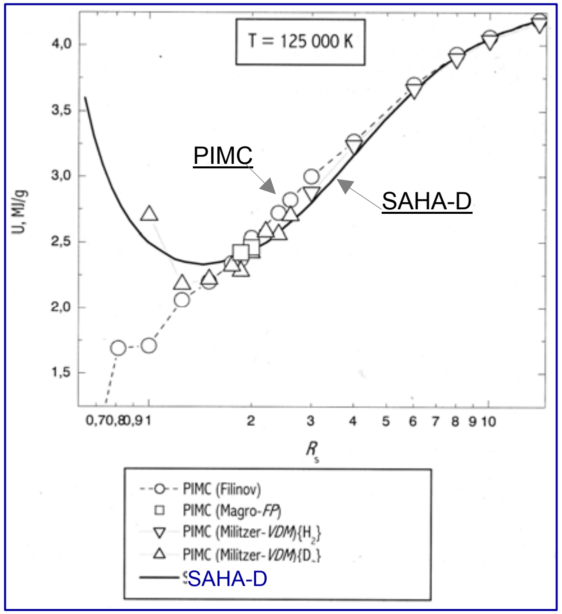


FIG. 4. Pressure-volume relations for solid hydrogen determined from x-ray diffraction at 300 K (Mao et al., 1988; Hem-





Isotherm T = 300 K

Comparison with experiment

Isotherm T = 5’000 K

Comparison with *non-empirical* atom-atomic approximation

Isotherm T = 125’000 K

Comparison with *ab-initio* approach

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

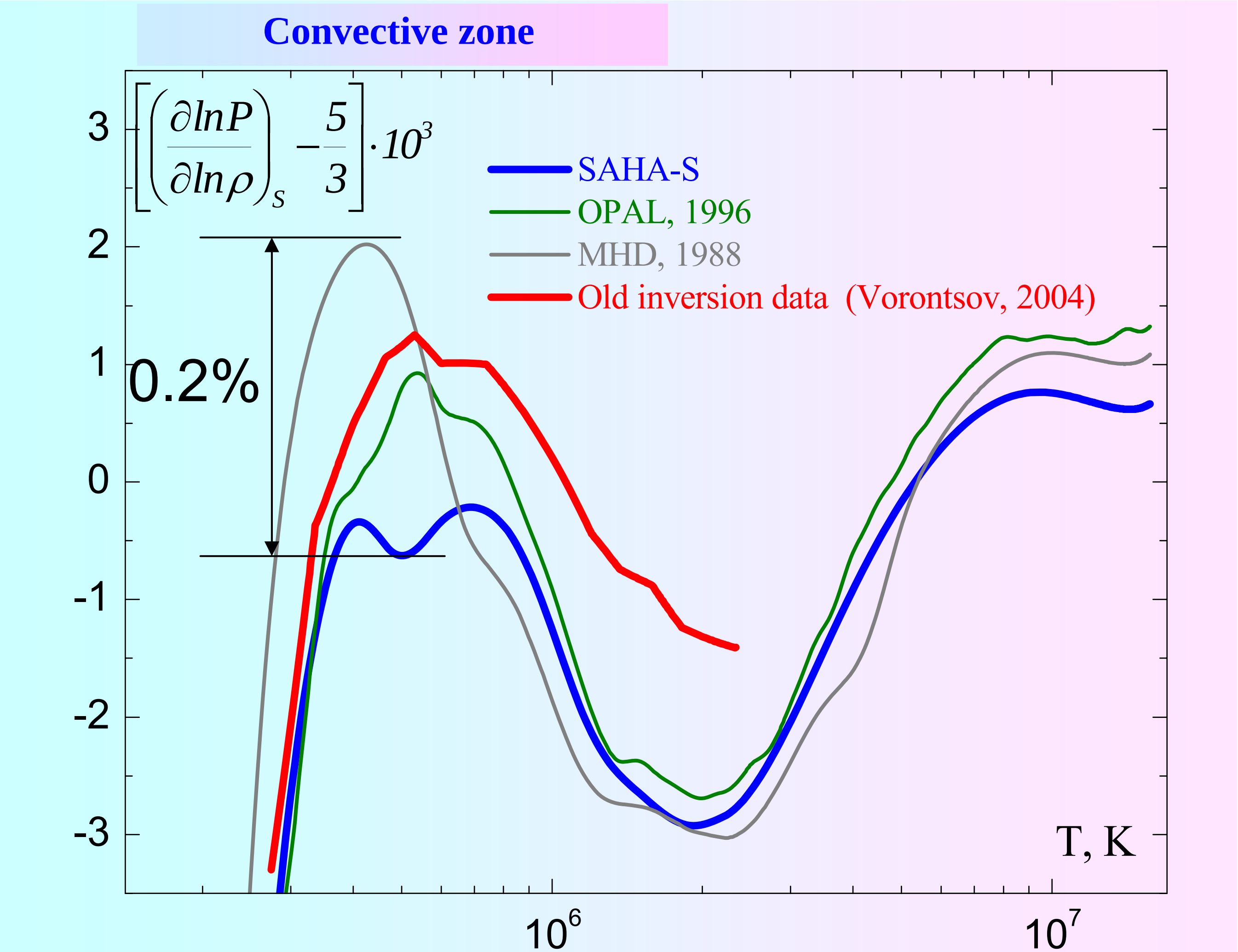
AAP -Yakub E.S. *Physica* B 265 31 (1999)

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

SAHA-S

Helioseismology

Models and old inversion data

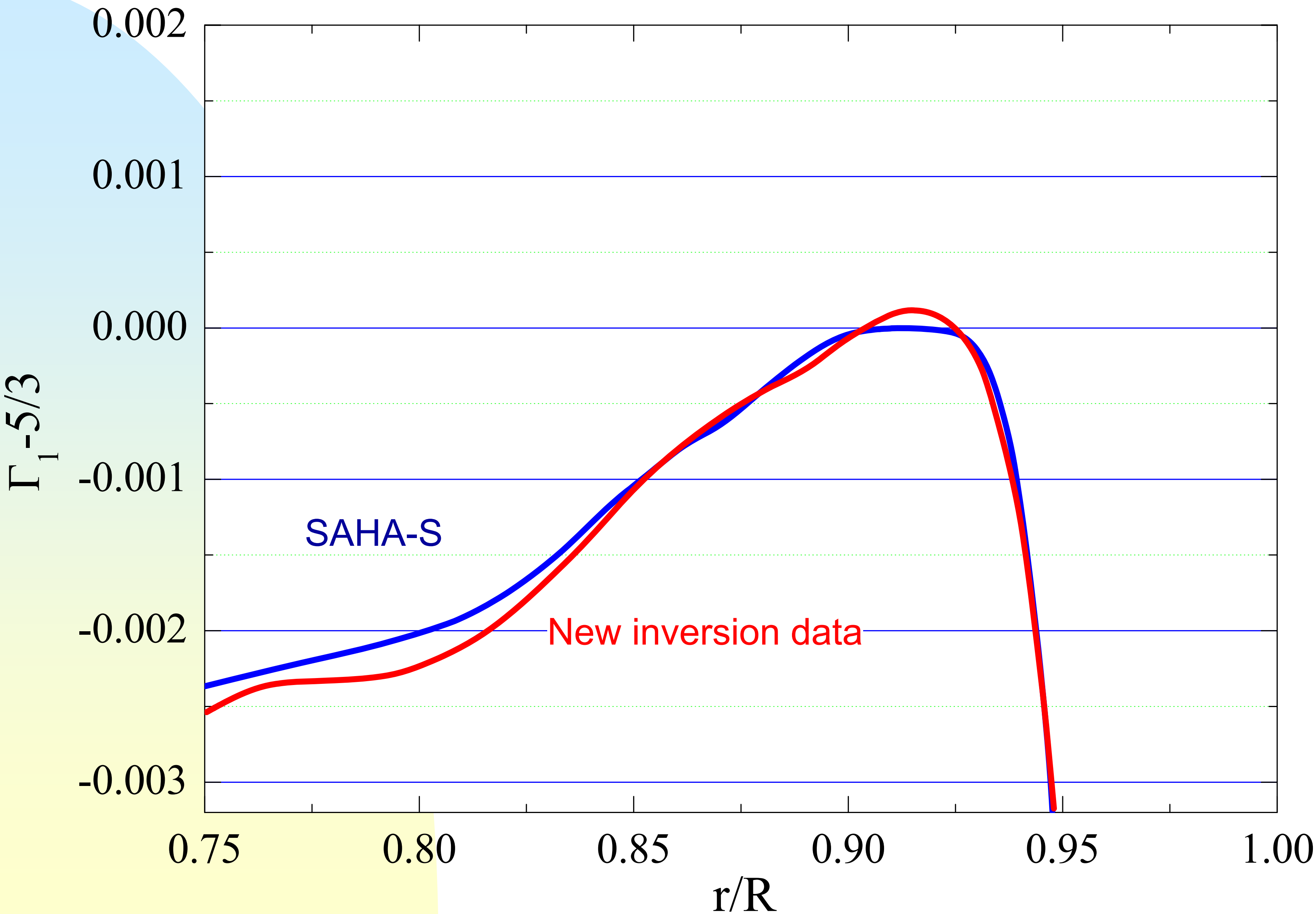


SAHA-S – asympthotically exact model for thermodynamics of solar plasma

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!