Ioffe Physical-Technical Institute

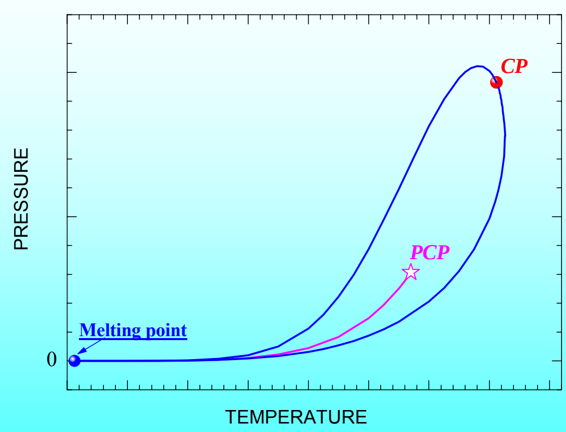
Department of Theoretical Astrophysics

April 17, 2007

NON-CONGRUENT PHASE TRANSITIONS IN INTERIORS OF GIANT PLANETS

Igor Iosilevskiy

Moscow Institute of Physics and Technology
(State University)



1967

Nature **215** (1967);

Internal Structure and Energy Emission of Jupiter

R. Smoluchowski

Princeton University Princeton, New Jersey

Jupiter emits much more energy than it absorbs. Explanations of the source of this heat depend upon our knowledge of its interior and of the behavior of condensed matter at very high temperatures and pressures.

1968 -1970

Norman & Starostin, *Plasma Phase Transition Concept*

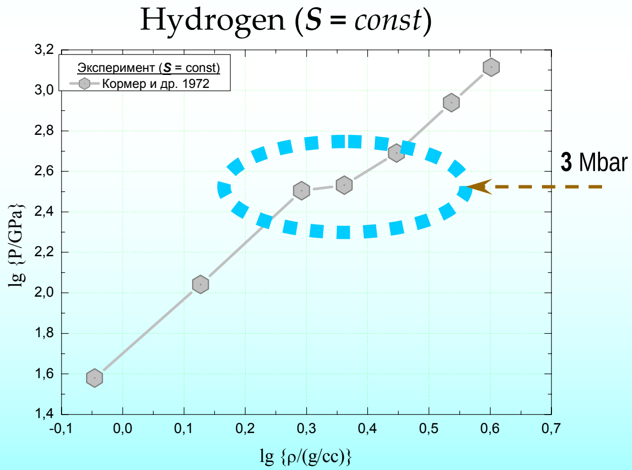
1972

Kormer et al. (Russian Nuclear Center (Sarov)),

Density jump in quasi-isentropic compression of hydrogen

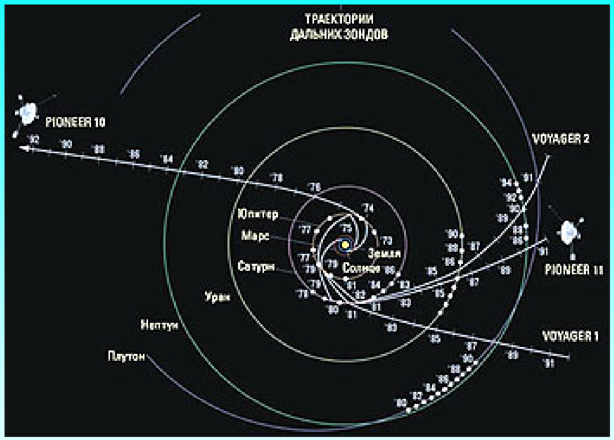
(P~ 3 Mbar)

? - Plasma Phase Transition - ?



1977

Voyager spacecrafts mission to Saturn



- Launch (1977)
- Start of Jupiter exploring (1979)
- Start of Saturn exploring (1980)
- Voyager mission is still valid (2007)

Phase Separation in Giant Planets:

Jonathan J. FORTNEY, William B. HUBBARD
Icarus, 164 (1) 2003

Atmospheric elemental abundances in Jupiter and Saturn
(*mass fractions*)

Element	SOLAR	JUPITER *Galileo*	SATURN *Voyager*	SATURN **revised**
H	0.736	0.742	0.92	0.76
He	**0.249**	**0.231** ± 0.04	**0.06** ± 0.05	**0.215** ± 0.035

1977

Stevenson & Salpeter, *Astrophysical Journal, Suppl.* **35** (1977)

- *The phase diagram and transport properties for hydrogen-helium fluid planets* (p.221-237)
- *The dynamics and helium distribution in hydrogen-helium fluid planets* (p.239-261)

1977

Iosilevskiy I., PhD Thesis, *"Non-congruent" condensation in $H_2 + Li$ plasma* (1977)

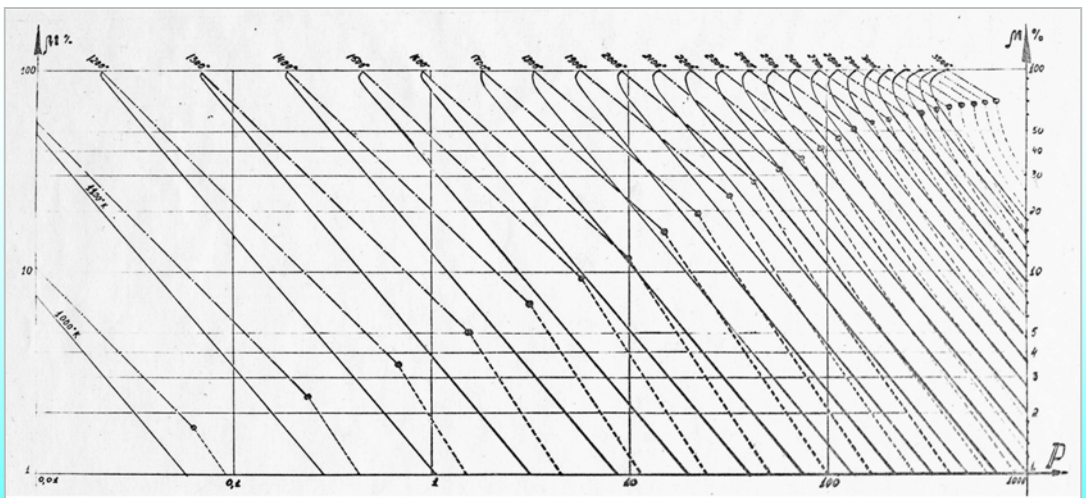


Рис. 37. Граница конденсации в смеси $H_2 + Li$. По оси ординат – мольная доля Li в смеси. Штриховые линии – выпадение в осадок гидрида лития; штрих-пунктирные – выпадение в осадок LiH ; сплошные линии – осадок считается идеальным раствором из Li и LiH

1989

Galileo spacecraft mission to Jupiter

- Launch (1989)
- Start of Jupiter exploring (1995)
- The end of Galileo mission (Sept. 21, 2003)

Phase Separation in Giant Planets:

Jonathan J. FORTNEY, William B. HUBBARD

Icarus, 164 (1) 2003

Atmospheric elemental abundances in Jupiter and Saturn

(*mass fractions*)

Element	SOLAR	JUPITER *Galileo*	SATURN *Voyager*	SATURN **revised**
H	0.736	0.742	0.92	0.76
He	0.**249**	**0.231** ± 0.04	**0.06** ± 0.05	0.**215** ± 0.035

1992

Strongly Coupled Plasma Physics

Int. Conference, Rochester // Chair: **Hugh Van Horn**

Chabrier, Saumon, Hubbard & Lunine
Ap.J **391** (1992)
The molecular-metallic transition of hydrogen and the structure of Jupiter and Saturn

= «» =

Saumon, Hubbard, Chabrier & Van Horn
Ap.J **391** (1992)
The role of the molecular-metallic transition of hydrogen in the evolution of Jupiter, Saturn, and brown dwarfs

Expected presence of «plasma phase transition» in interiors of Jupiter and Saturn

(Chabrier G., Saumon D., Hubbard W., Lunine J. *Astrophys. Journal* **381** (1992) p.817)

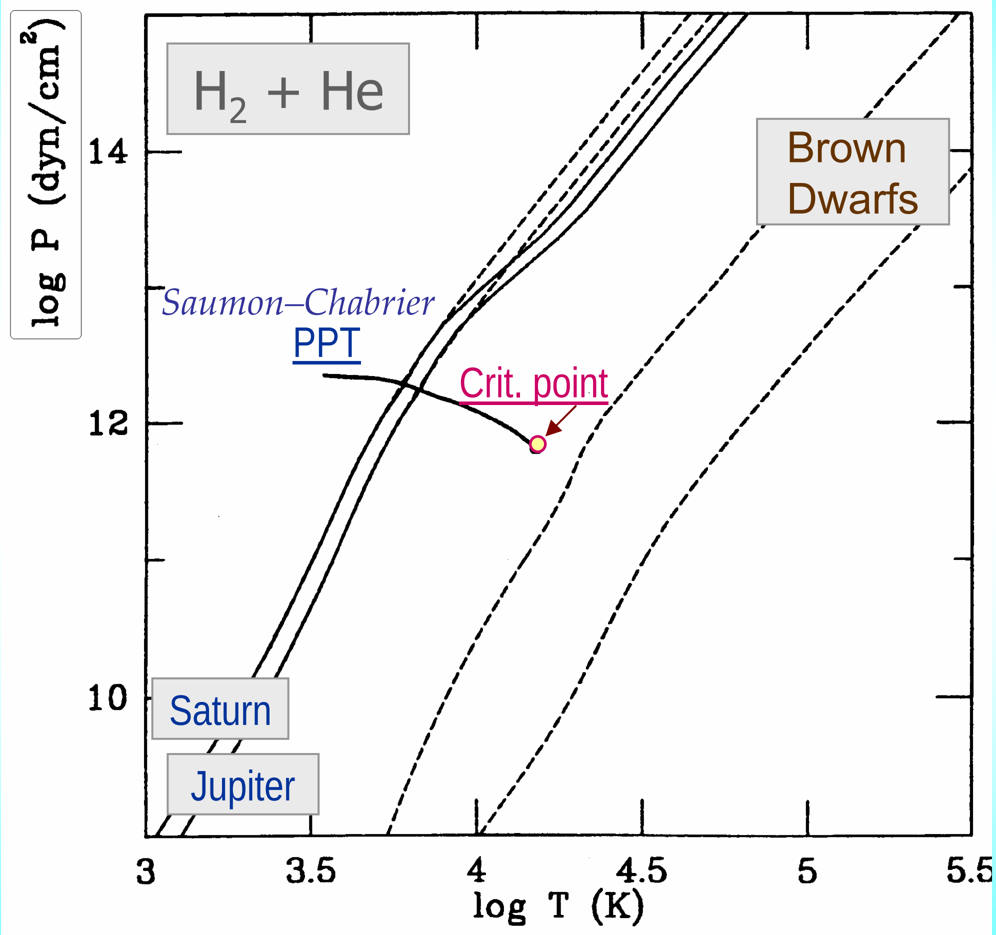


FIG. 3.—Adiabats computed from the EOS described in § 2 with a helium mass fraction $Y = 0.24$. The heavy solid line is the coexistence curve of the plasma phase transition and the critical point is indicated by a dot. Solid lines are computed from the EOS with PPT, dashed lines from the interpolated hydrogen EOS (see text). The temperature of the adiabats at the 1 bar pressure level is, from left to right: 135 (Saturn), 165 (Jupiter), 1500, and 3500 K. In a

1992

Strongly Coupled Plasma Physics

Int. Conference, Rochester // Chair: **Hugh Van Horn**

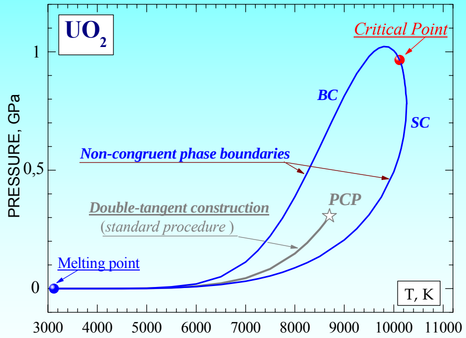
1992

Launch of INTAS-93-66 Project, *Equation of State of Uranium Dioxide up to the Critical Point*

1997

Finish of the first stage of INTAS Project

Conference on EOS of matter under extreme conditions, Elbrus



1997 - 2007

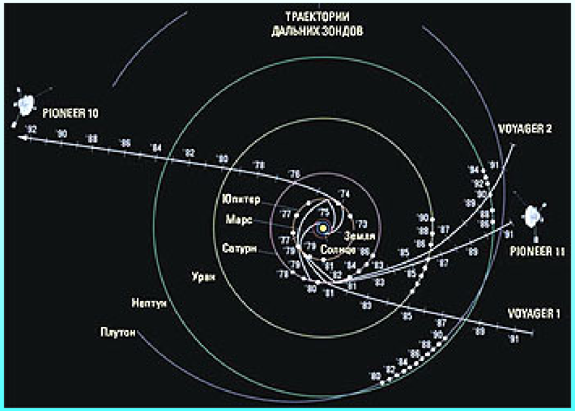
Cassini-Huygens mission to Saturn

-Launch (*Oct. 1997*)

Perturbation maneuvers

- Venus-2 (*April 1998, June 1999*)
- Earth (*August 1999*)
- Jupiter (*December 2000*)

- Start of Saturn Exploring (*June, 2004*)



June **2004**

Start of Saturn exploring by Cassini-Huygens

June **2004**

Iosilevskiy I., *Non-congruent phase transitions in astrophysical objects*

International Workshop

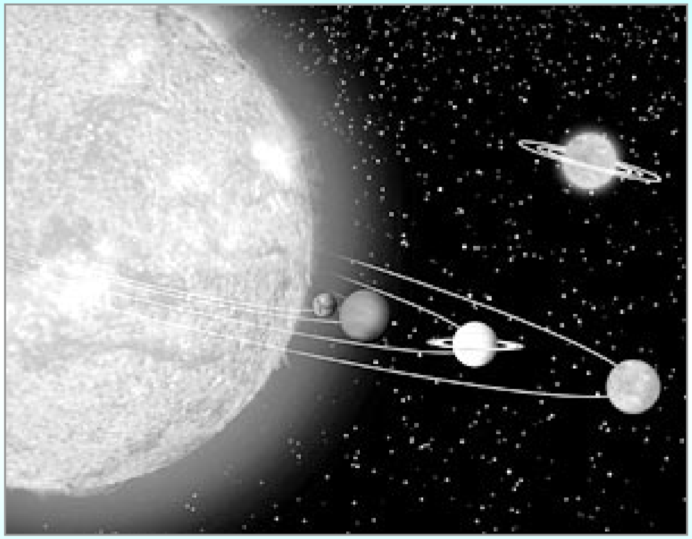
Equation-of-State and Phase-Transitions in Ordinary Astrophysical Matter

Leiden, Lorentz Center

(June, 2004)

Dominating hypothesis:

Jupiter & Saturn were formed simultaneously (~ 4,5 GYr) from the protoplanetary plasma with composition similar to protosolar



Phase Separation in Giant Planets:
Inhomogeneous Evolution of Saturn

Jonathan J. FORTNEY, William B. HUBBARD
(*Lunar and Planetary Laboratory, University of Arizona*)

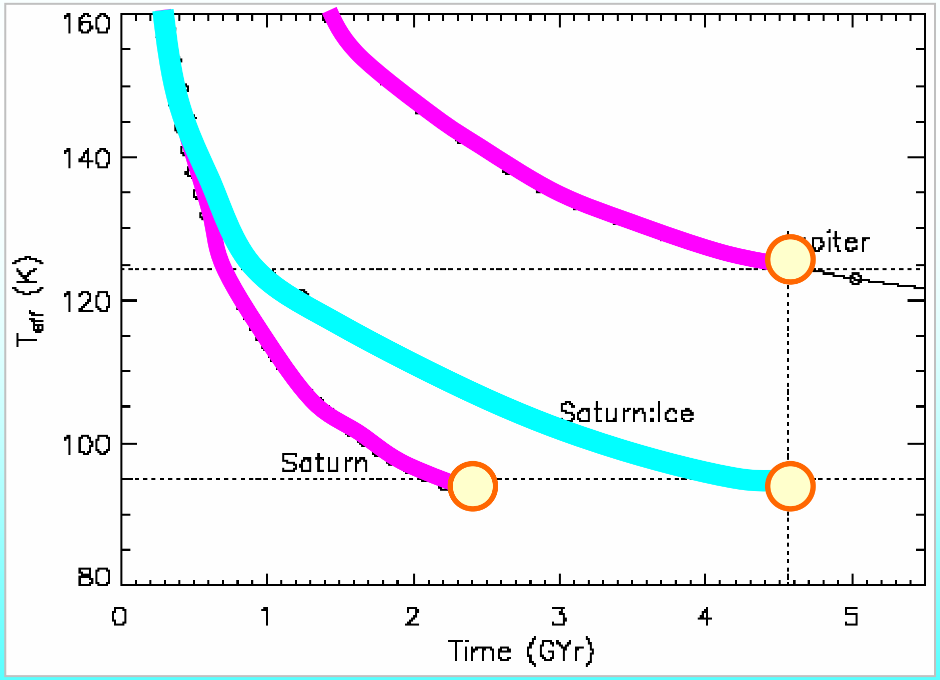
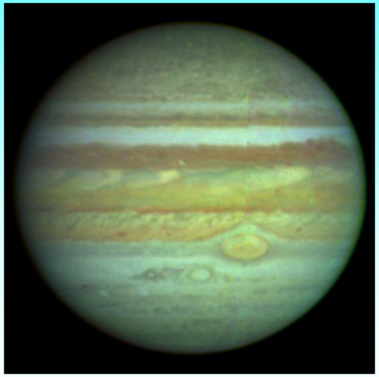
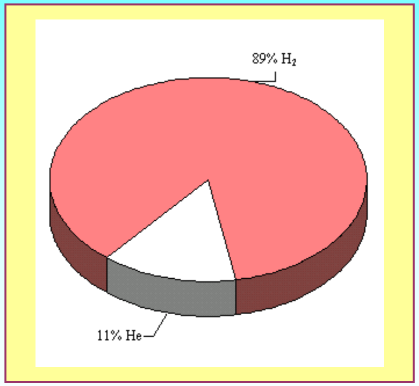
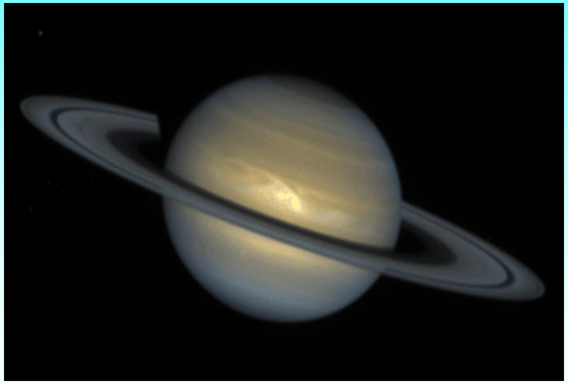


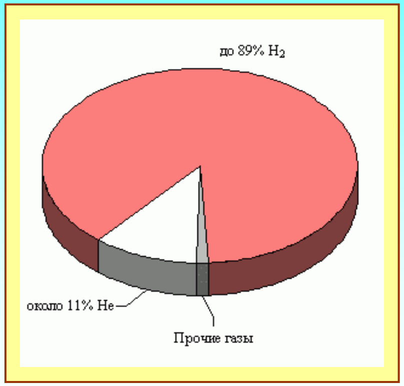
Figure 14. Evolution of Saturn with separation of heavy elements. Homogeneous evolutionary models are labeled "Saturn" and "Jupiter," while the evolution of Saturn with separation of CNO elements is labeled "Saturn:Ice." The

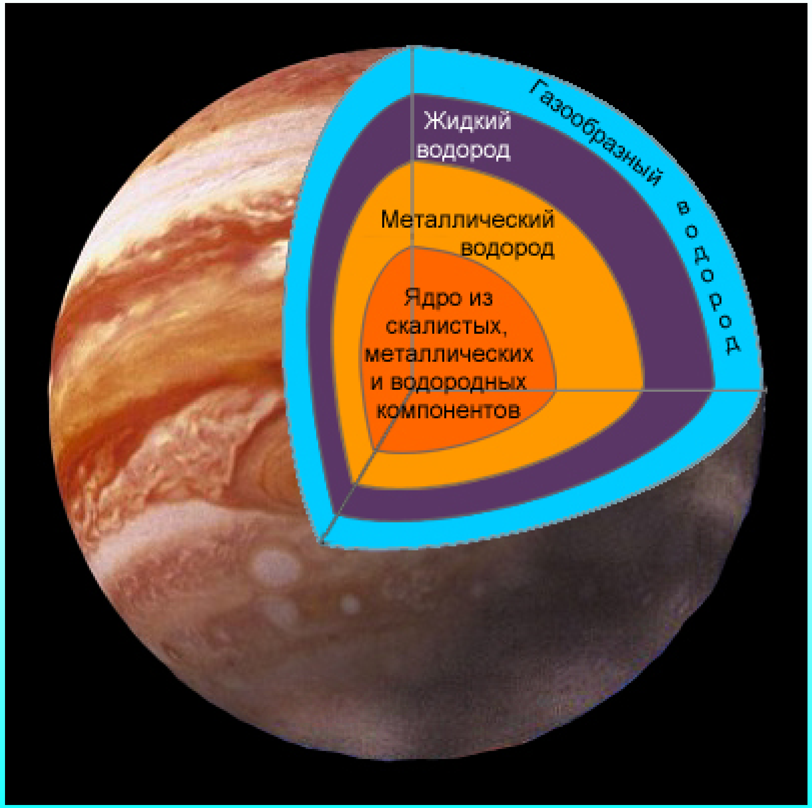
Hypothetical phase transitions in interiors of Jupiter and Saturn

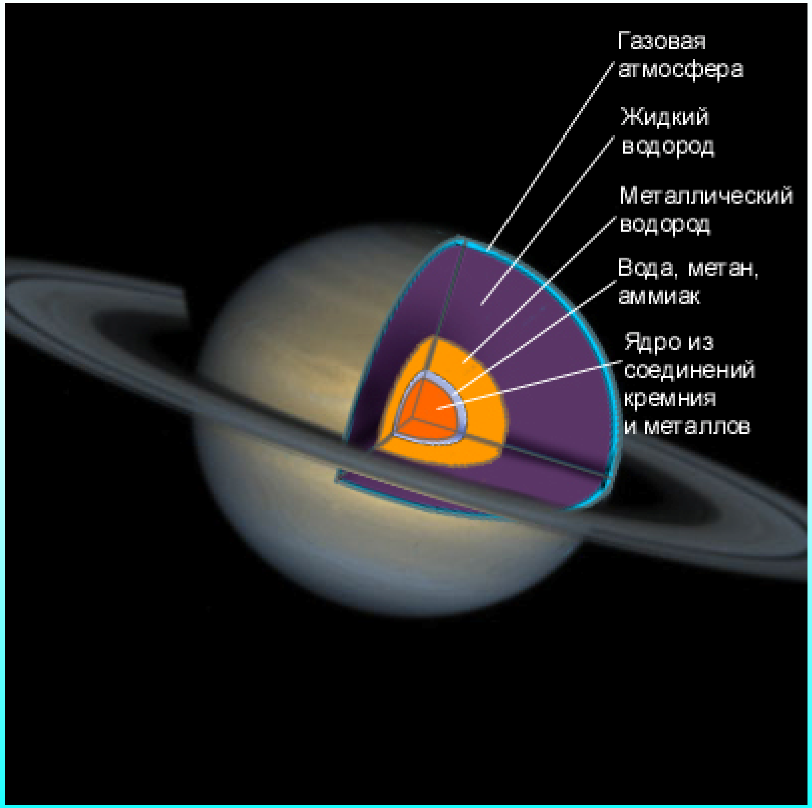






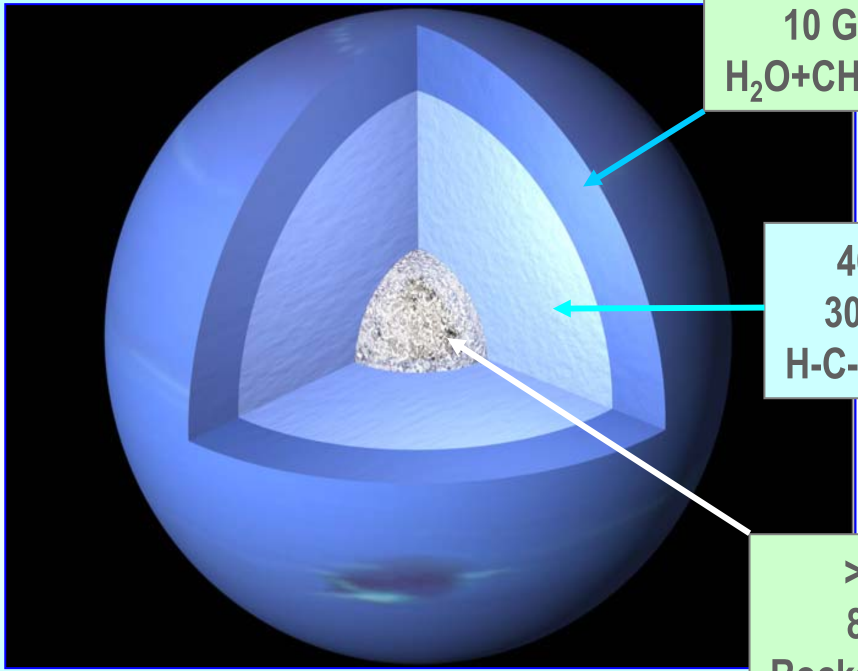






Hypothetical Phase Transitions in interiors of Solar System Giant Planets

Neptune

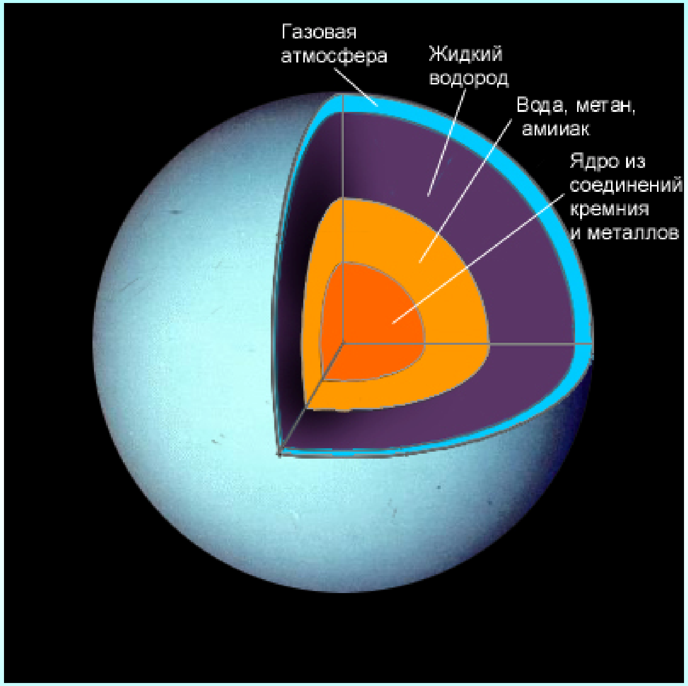


2000 K
10 GPa
$H_2O+CH_4+NH_3$

4000 K
300 GPa
H-C-N-O ices

> 5000 K
800 GPa
Rocks, diamond?

Uranus



More than 200 «extrasolar» giant-planets have been discovered

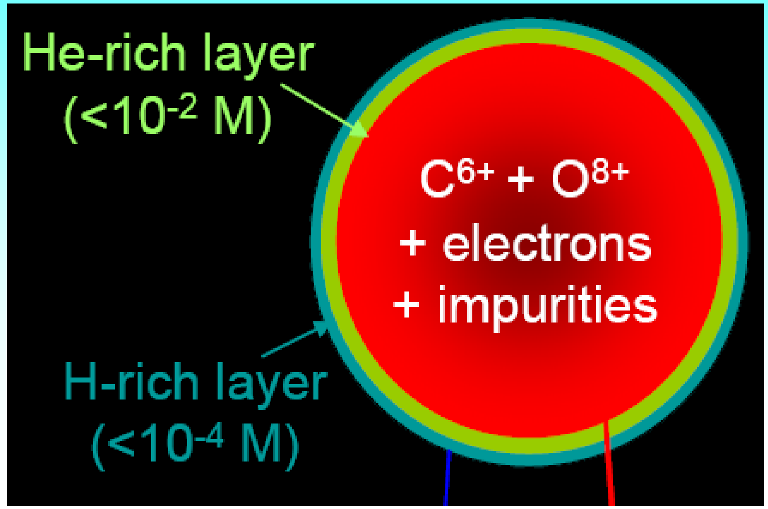
("Hot Jupiters")

EGP–33634

Уже открыто более 200 «внесолнечных» планет–гигантов

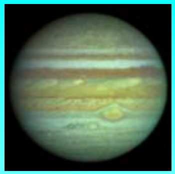
(«горячие Юпитеры»)

Hypothetical phase transitions in outer layers of white dwarfs



Jérôme Daligault // SCCS, Moscow, 2005

^{22}Ne



Phase transitions in H_2 + He mixture

"**Helium rain**" (**?**)
Hypothetical demixing of He and H_2
in upper and inner layers of Jupiter and Saturn

Immiscibility gap in H_2/He mixture

- Low-temperature demixing of ***liquid*** H_2 and He in ***upper*** layer of **J** and **S**
- High-temperature demixing of ***ionized*** H and He in ***inner*** layer of **J** and **S**

Phase transitions in H_2/He mixture

transformed from their **prototypes** in pure hydrogen and helium:

- ***hydrogen-like*** phase transition(s)
- ***helium-like*** phase transition(s)

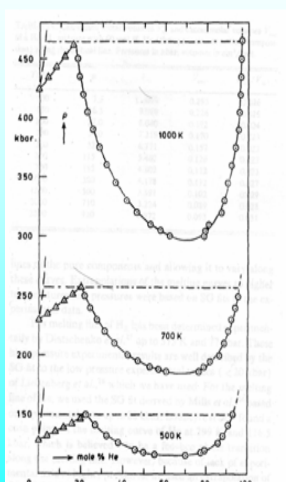
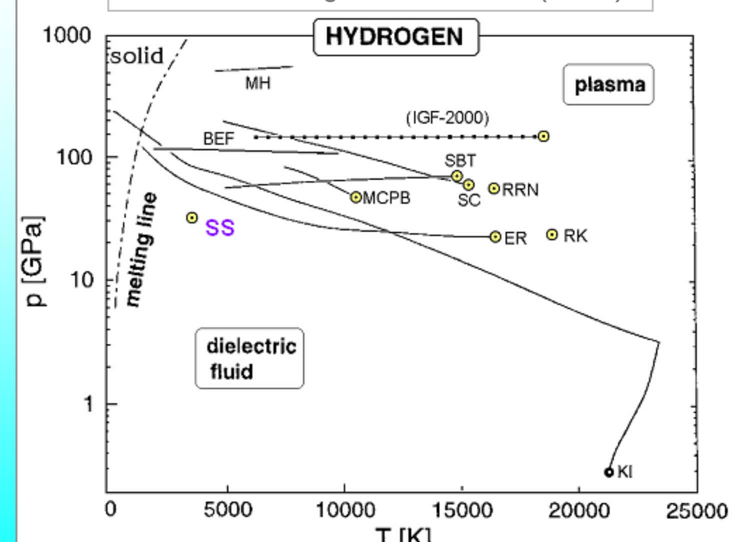


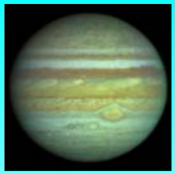
FIG. 4. Calculated fluid–fluid and solid–fluid isotherms at 500, 700, and 1000 K. Dashed-dotted lines represent solid–fluid–fluid three-phase equilibrium.

Coexistence of fluid He and H_2
(*theory vs. experiment*)

Loubeyre P., Toullec R., Pinceaux J. *Phys. Rev. B* **36**, 3723 (**1987**)
Van den Bergh L., Schouten J. *J. Chem. Phys.* **89** (4) 2336 (**1988**)
Schouten J., de Kuijper A., Mishel P. *Phys. Rev. B* **44**, 6330 (**1991**)

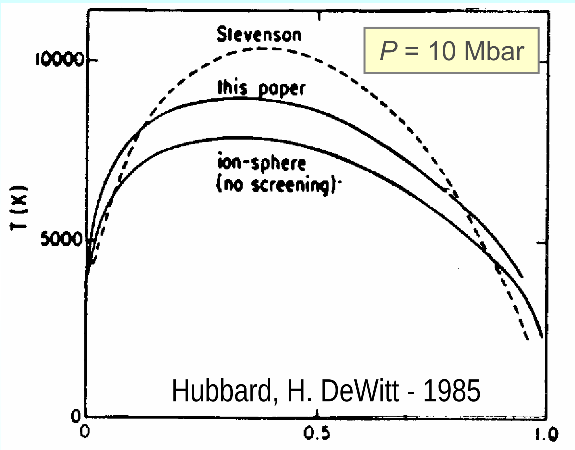
Beulle, Ebeling *et al*. *PRB* **59** (1999)



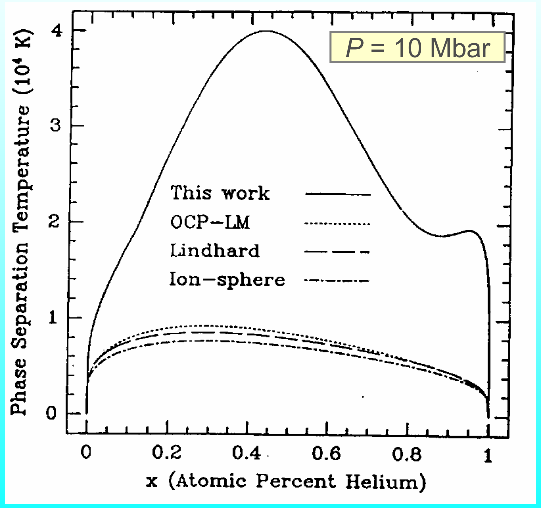


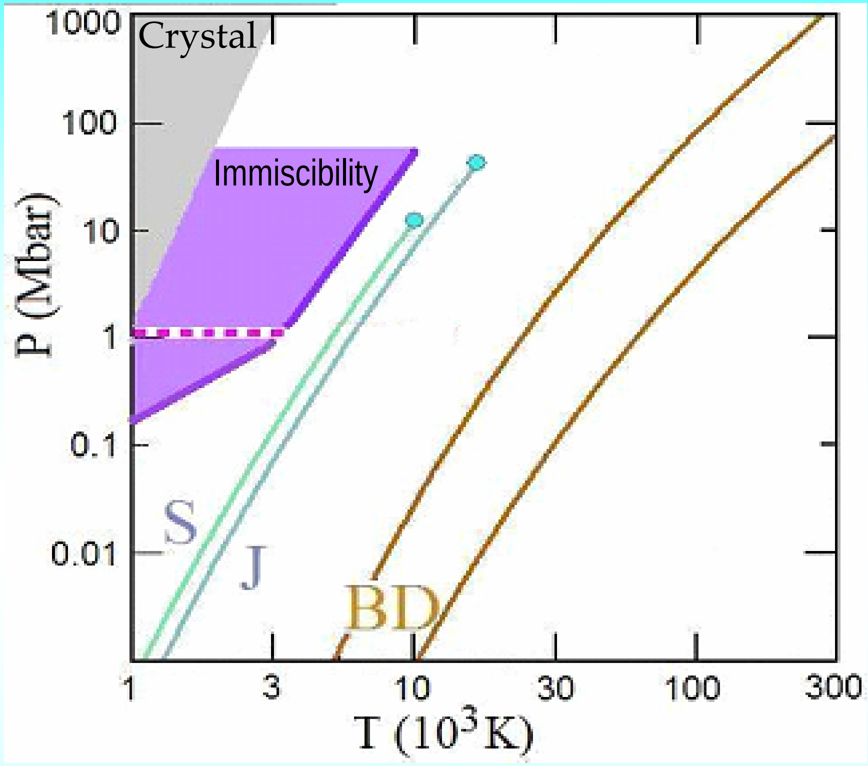
Phase decomposition in H + He mixture

"**Helium rain**" (?)
Hypothetical demixing of ionized H and He in inner and upper layers of Jupiter and Saturn



Ross *et al.* 1991





Calculation of demixing boundary for H / He plasma
{ $H^{+} + He^{++} + e(-)$ }
via Density Fuctional Theory (DFT) + Mol.Dynamics:

Pfaffenzeller O., Hohl D., Ballone P. *Phys.Rev.Lett.* **74, 2599 (1995)**

D. Stevenson, E. Salpiter, *Astrophysical Journal* **35,** 221 **(1977)**
W. Hubbard, H. DeWitt, *Astrophysical Journal,* **290,** 388 **(1985)**
M. Ross, J. Klepeis, K. Shafer, T. Barbee III - *Science,* **254** 986 **(1991)**
SCCS Conference, Rochester, **(1993)**

Expected presence of «plasma phase transition» in interiors of Jupiter and Saturn

(Chabrier G., Saumon D., Hubbard W., Lunine J. *Astrophys. Journal* **381** (1992) p.817)

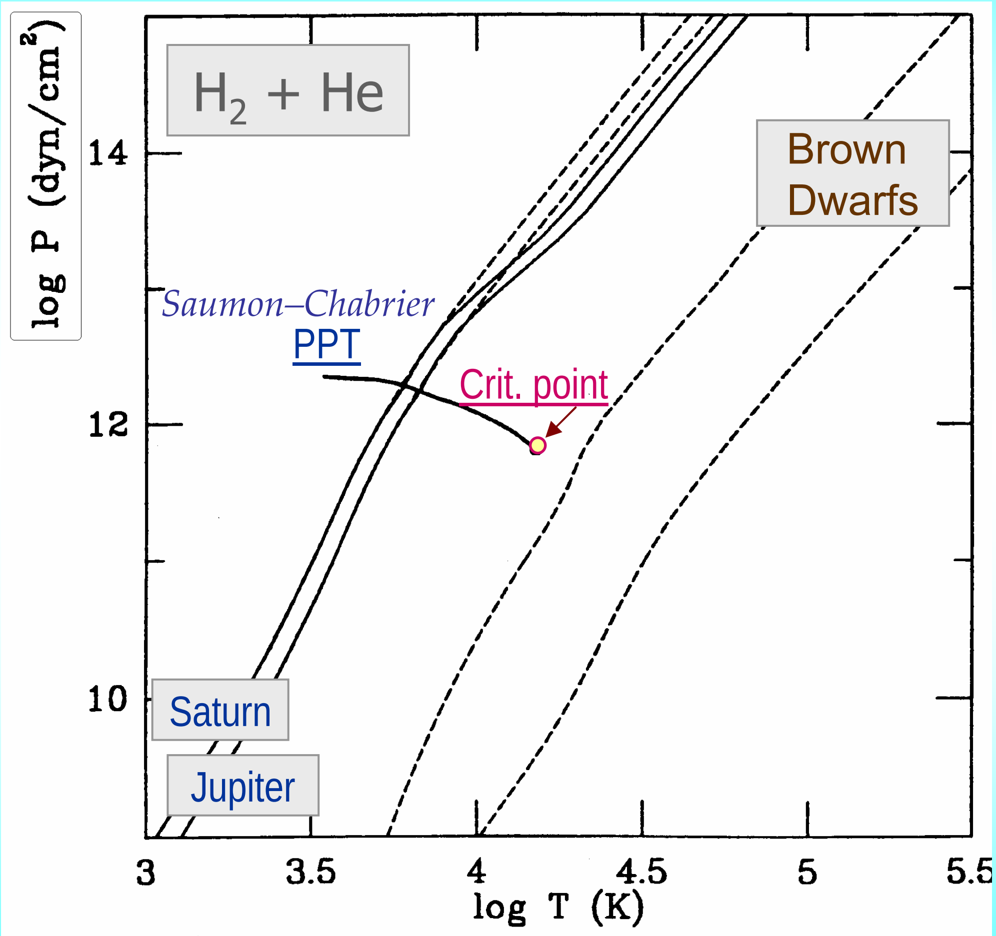
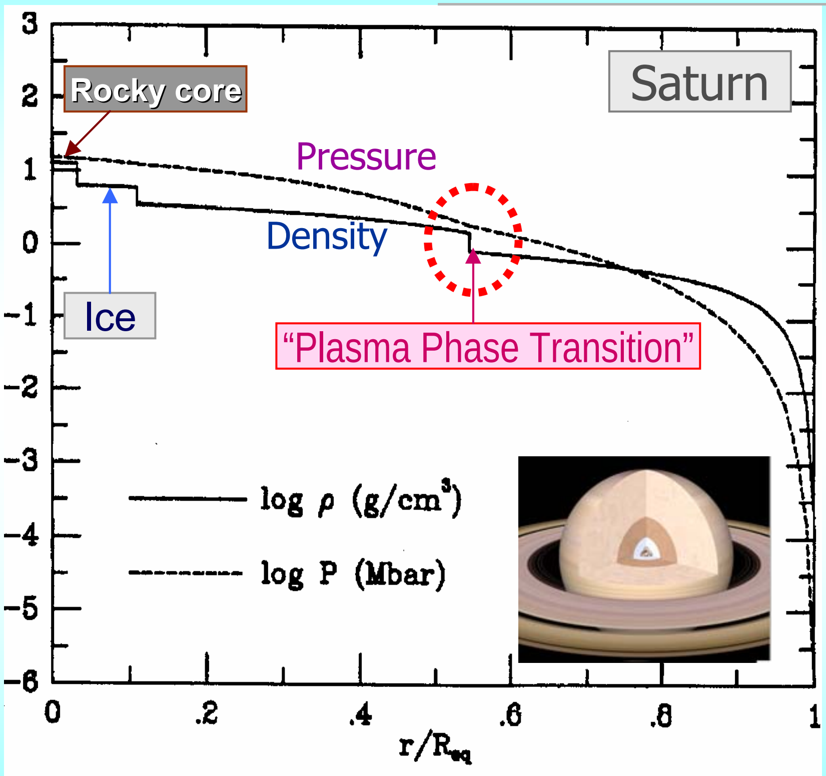


FIG. 3.—Adiabats computed from the EOS described in § 2 with a helium mass fraction $Y = 0.24$. The heavy solid line is the coexistence curve of the plasma phase transition and the critical point is indicated by a dot. Solid lines are computed from the EOS with PPT, dashed lines from the interpolated hydrogen EOS (see text). The temperature of the adiabats at the 1 bar pressure level is, from left to right: 135 (Saturn), 165 (Jupiter), 1500, and 3500 K. In a

Typical picture of plasma phase transition expected in H_2/He mixture in interior of Jupiter and Saturn

Chabrier G., Saumon D., Hubbard W., Lunine J. (SCCS-1992, Rochester)



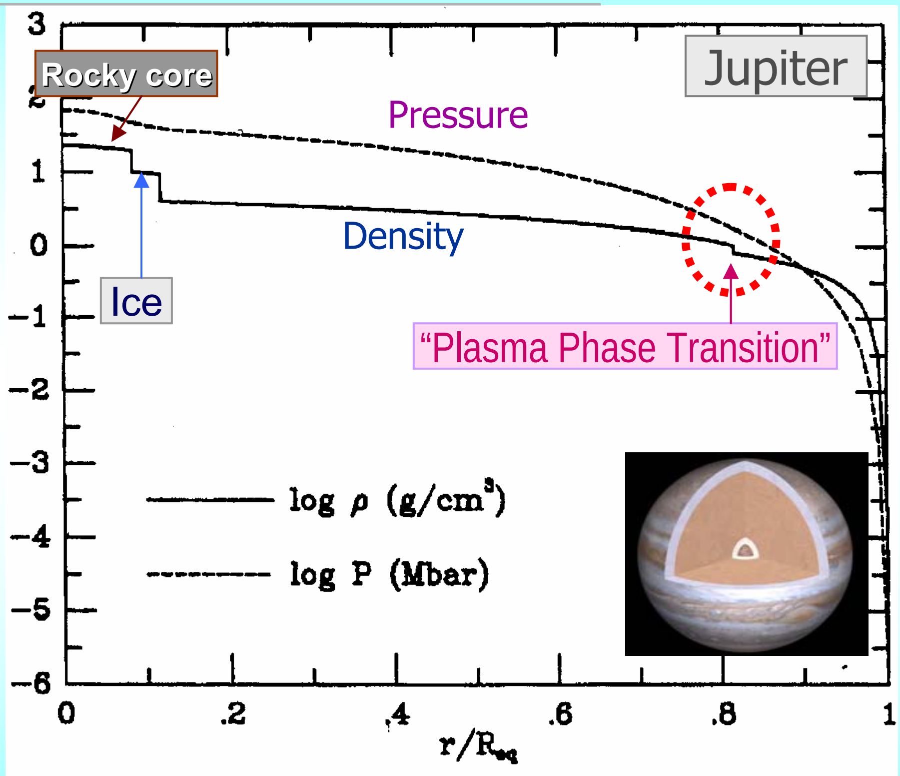


Fig. 1. Pressure and density profiles of optimized models of Jupiter (top panel) and Saturn (bottom panel), plotted as a function of mean radius. Discontinuities in the density clearly mark the boundaries of the four layers of the models: rocky core, ice mantle, metallic and molecular

Typical picture of plasma phase transition expected in interior of Giant Planets

Jupiter

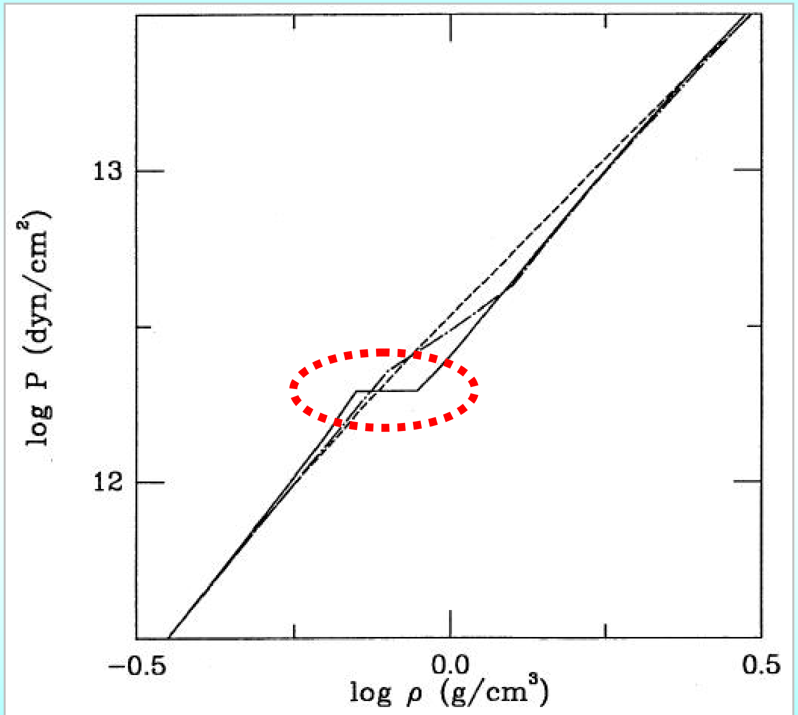


FIG. 2.—Pressure-density relation along a pure hydrogen Jupiter adiabat ($T = 165$ K at $P = 1$ bar). The MH EOS is shown by the long dash-dot curve,

GIANT PLANETS AND THE PLASMA PHASE TRANSITION OF HYDROGEN
D. Saumon, G. Chabrier, W. B. Hubbard, and J. I. Lunine 111

Neptune

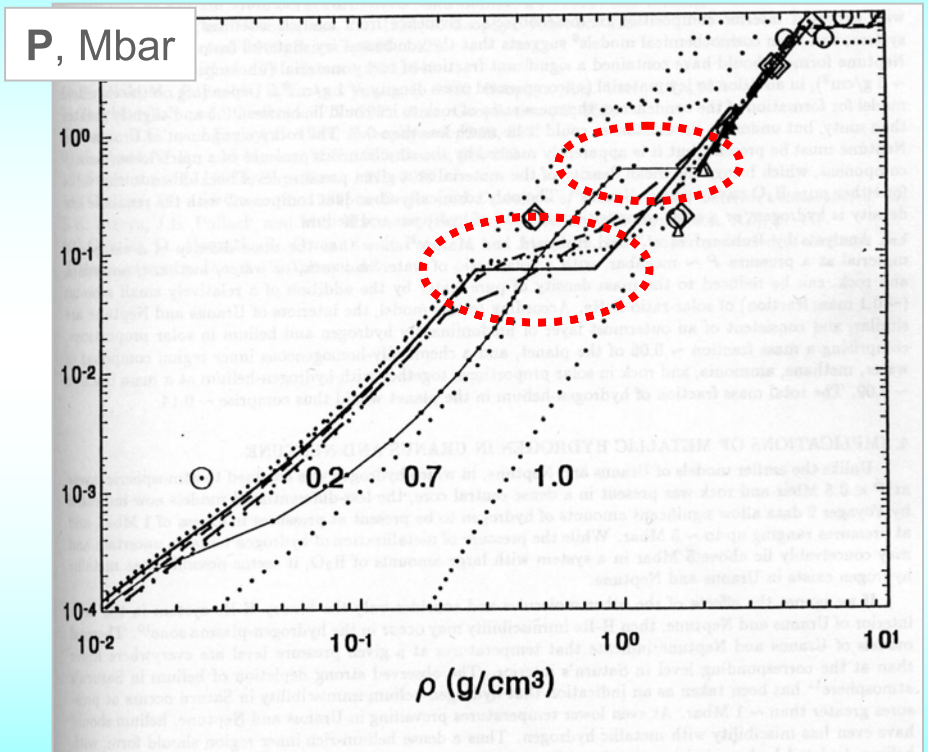
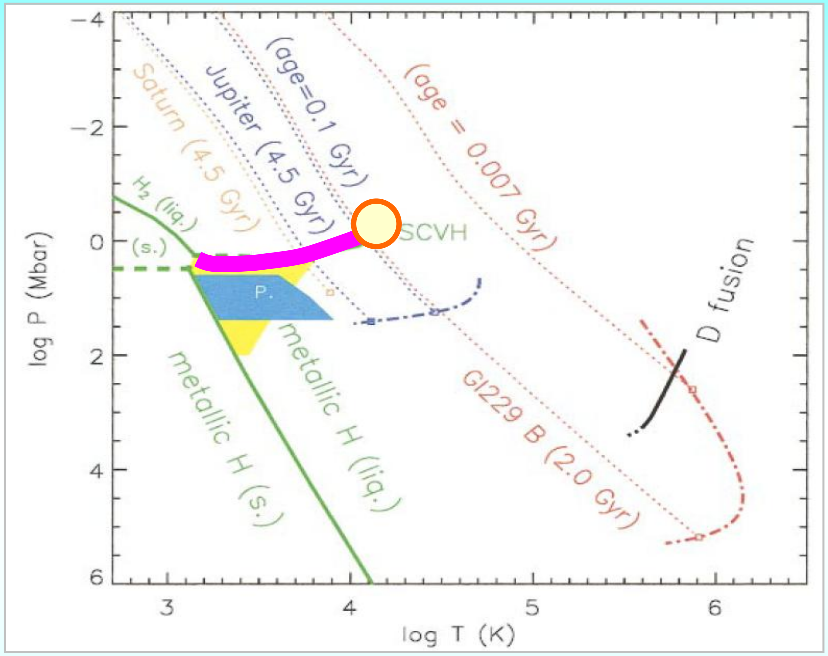


FIGURE 3
Pressure-density relations for Uranus and Neptune models, compared with theoretical curves. Dotted

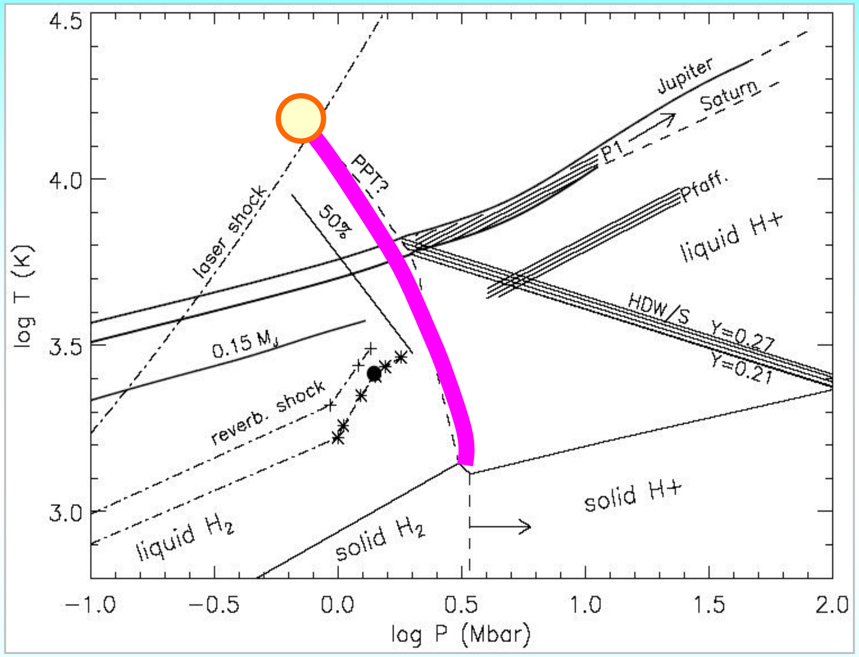
STRONGLY COUPLED PLASMAS IN URANUS AND NEPTUNE
W. B. Hubbard 131

Strongly Coupled Plasma Physics
Int. Conference, Rochester, 1992

Typical picture of plasma phase transition expected in interior of Giant Planets



BURROWS, HUBBARD, LUNINE and LIEBERT
The theory of brown dwarfs and extrasolar giant planets
Rev. Mod. Phys. 73, 719-769, 2001



J. FORTNEY & W. HUBBARD
Phase Separation in Giant Planets
Icarus, 164, 2003

Hypothetical “Plasma Phase Transition” in hydrogen

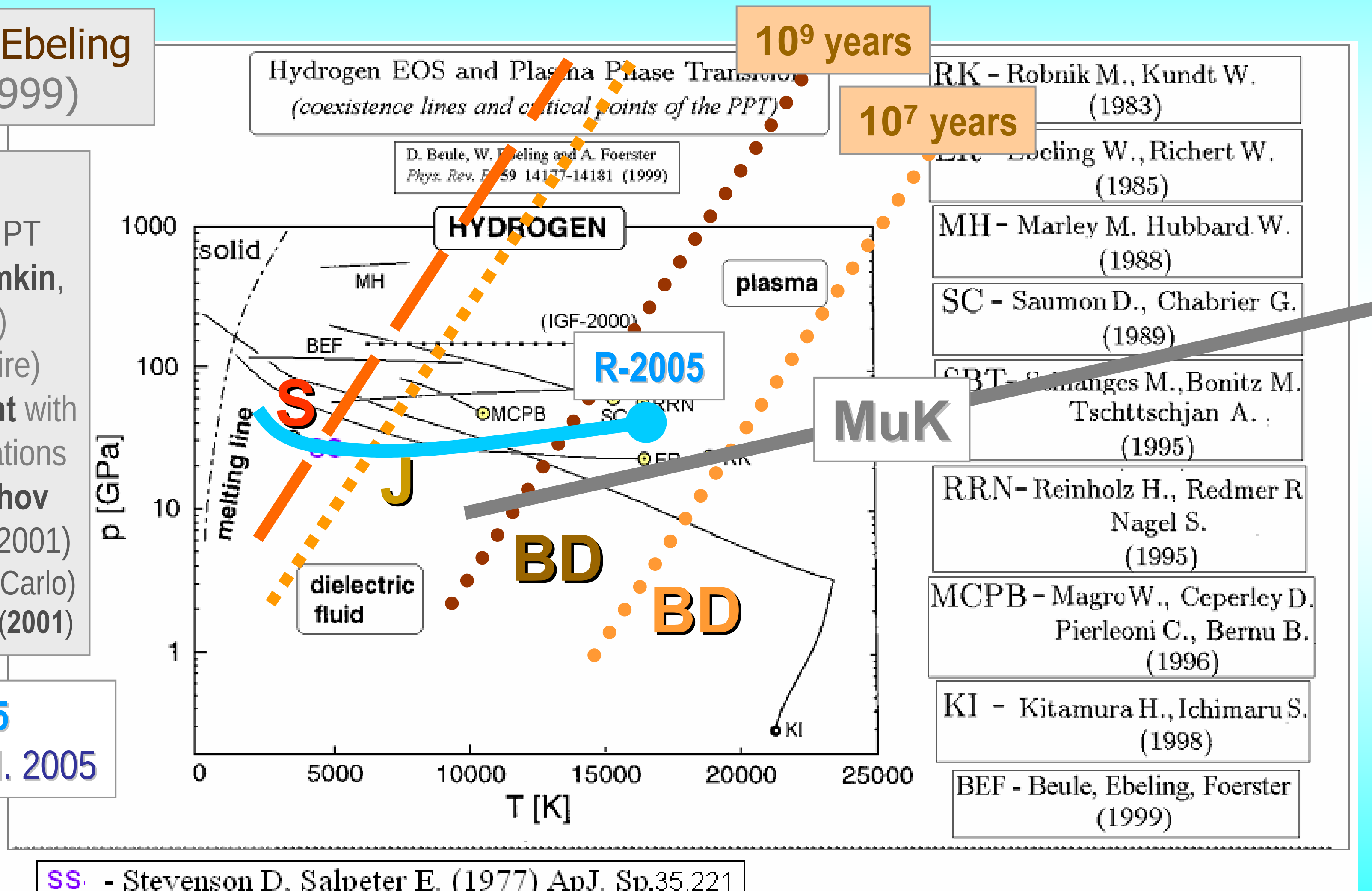
Relevant to the problem of Saturn and Jupiter formation

(*) Beulle, Ebeling *et al.* (1999)

“ **MuK** ”
“Dissociative” PT
Mulenko, **Khomkin**, *et al.* (2001)
(chemical pictire)

Good agreement with *ab initio* calculations
Filinov, Levashov
Bonitz, Fortov. (2001)
(Quantum Monte-Carlo)
Phys. Lett. A 289 (**2001**)

R-2005
Redmer et al. 2005



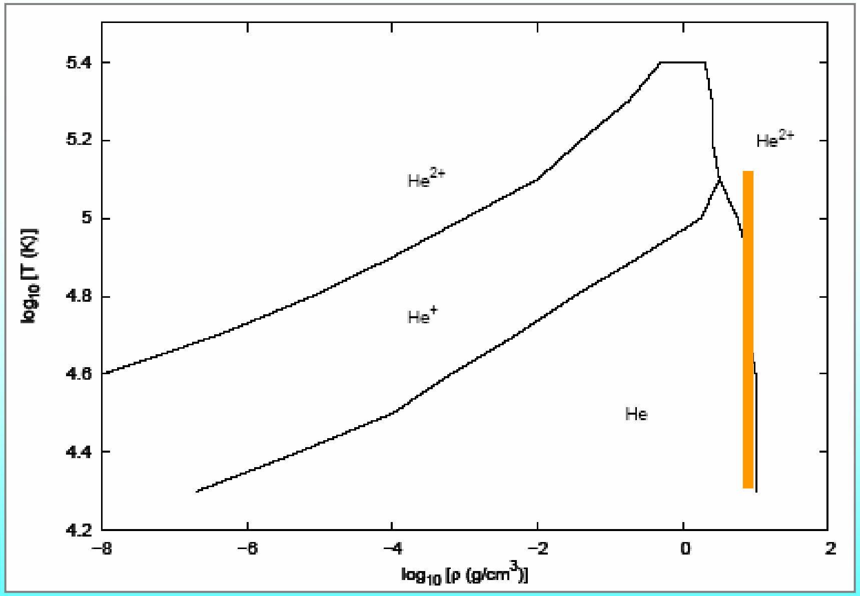
S – **Saturn**
J – **Jupiter**
BD – **Brown Dwarfs**

Hypothetical Plasma Phase Transition (transitions) in helium

Ebeling, Foerster *et al.* (1991)

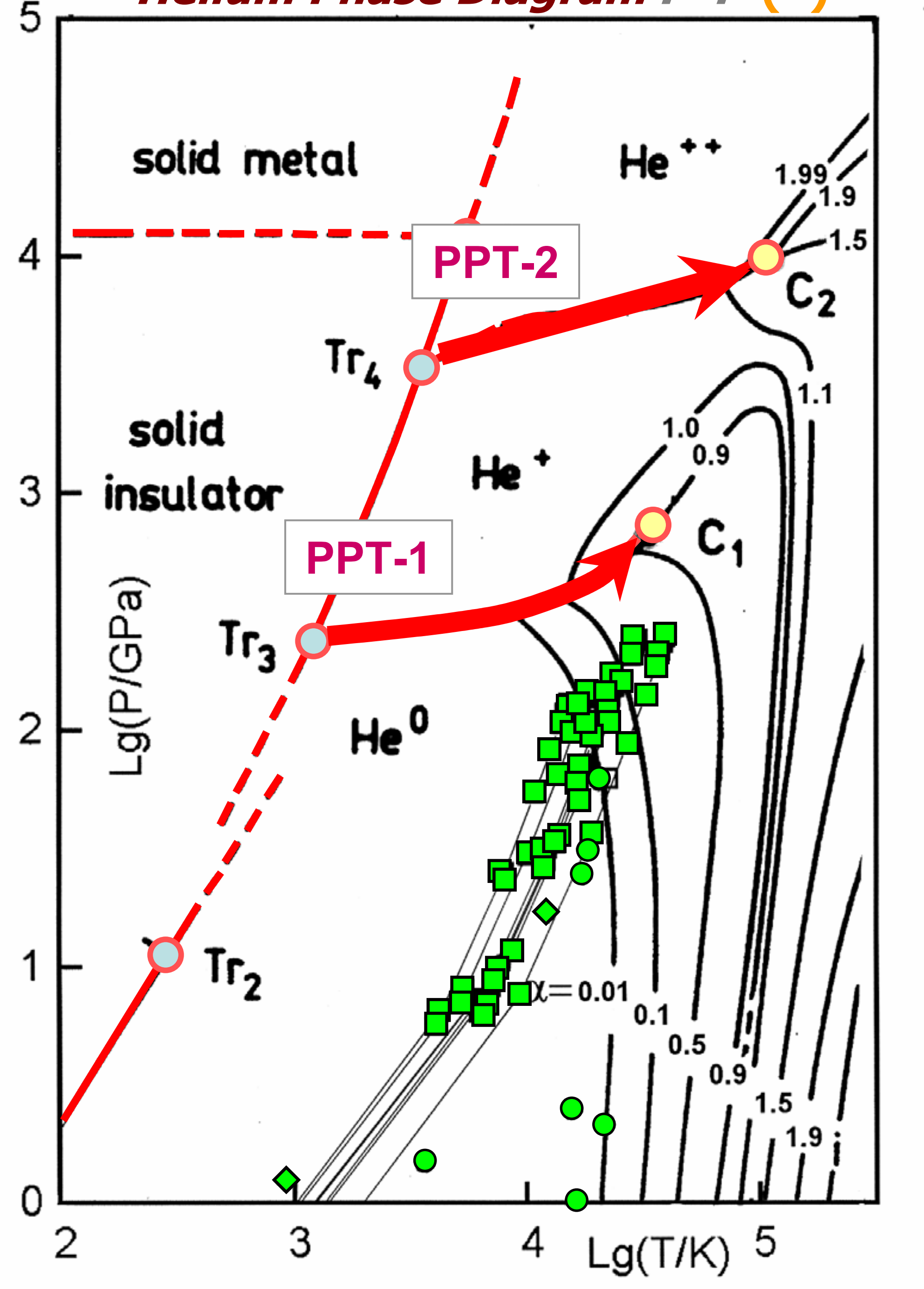
* * * * * * * * * * *

PPT?



Winisdoerffer Ch., Chabrier G.,
Free-energy model for fluid helium at high density
Phys.Rev.E (2005)

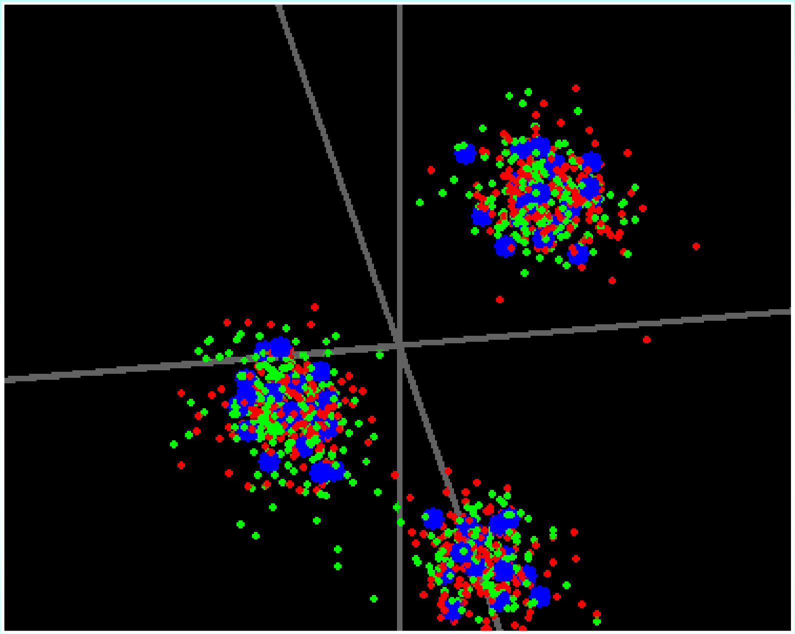
Helium Phase Diagram P-T (*)

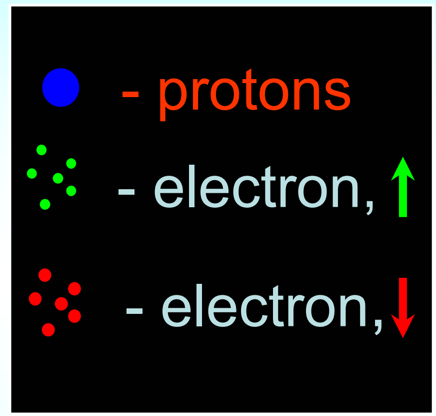


Quantum Monte-Carlo Simulations

(V. Filinov, M. Bonits, P. Levashov, V. Fortov)

"Plasma" phase transition in hydrogen





T = 10000 K, n = $3 \cdot 10^{22}$ cm^{-3}

Figure from:
V. Filinov,
P. Levashov
et al.
SCCS-2005,
Moscow

V. Filinov, M. Bonits, P. Levashov, V. Fortov
Phase Transition in Hydrogen Plasma
Pis'ma JETF **(2001);** ***J. Phys.*** **(2003);** ***Phys. Rev. E*** **(2004)**

Theoretical prediction of "dissociative" fluid-fluid phase transition in liquid hydrogen (deuterium)

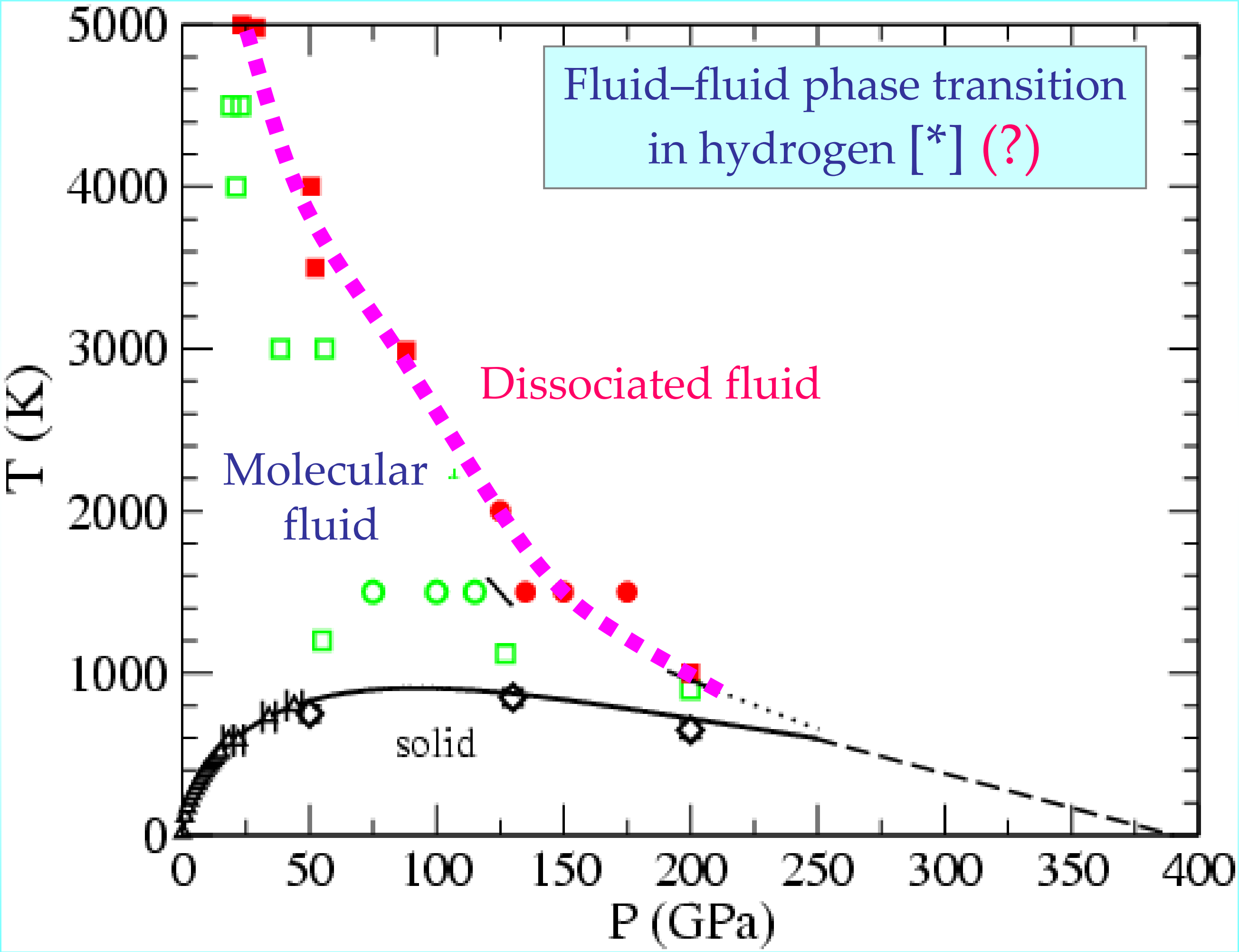


Figure from:
Giulia Galli,
SCCS-2005,
Moscow

Density Functional Theory + Molecular Dynamics

[*] Scandolo S. *PNAS* **100**, 3051 (2003) // Bonev S., Militzer B., Galli G. *PRB* (2004)

Theoretical prediction of "dissociative" fluid-fluid phase transition in liquid hydrogen

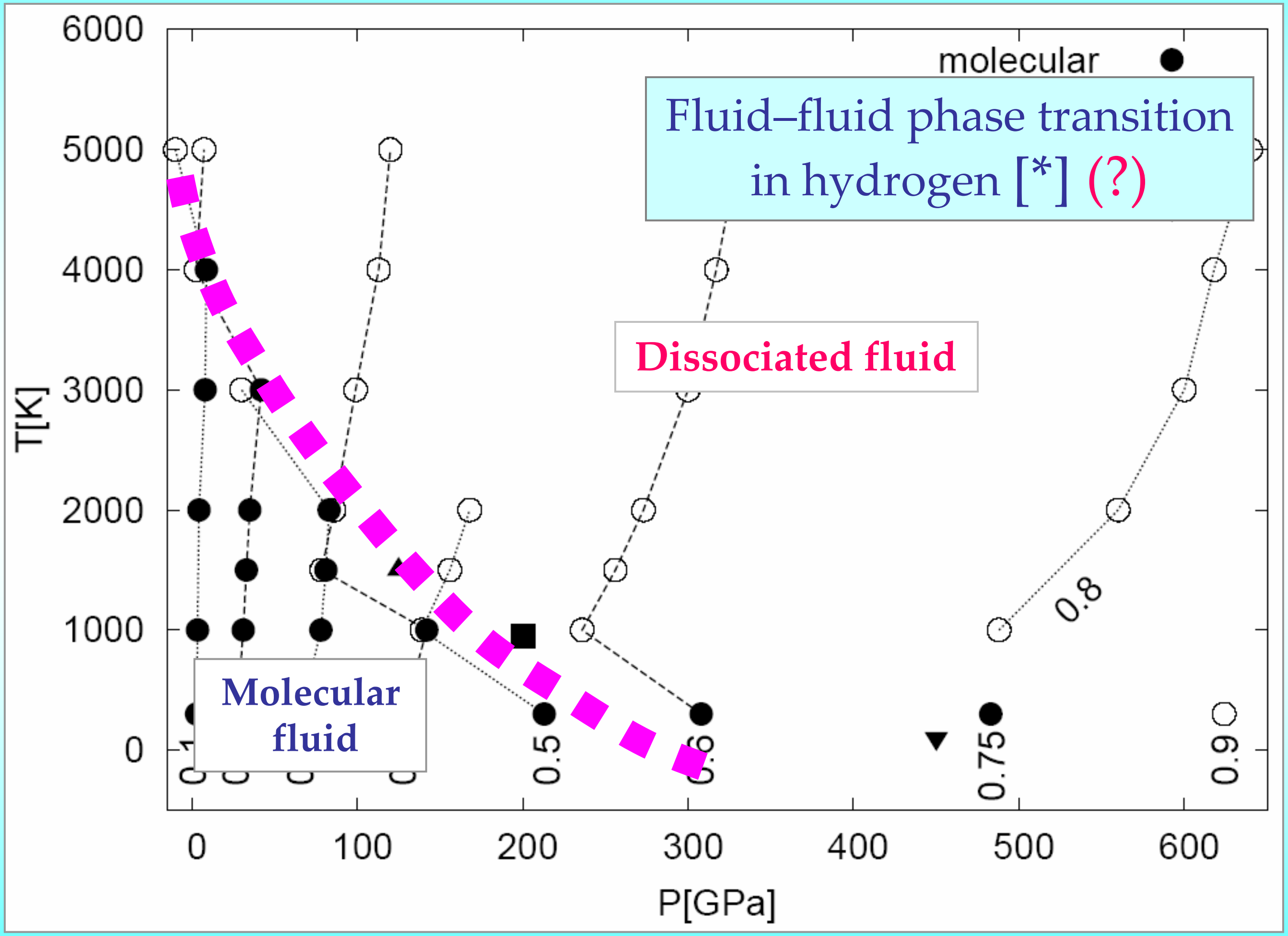


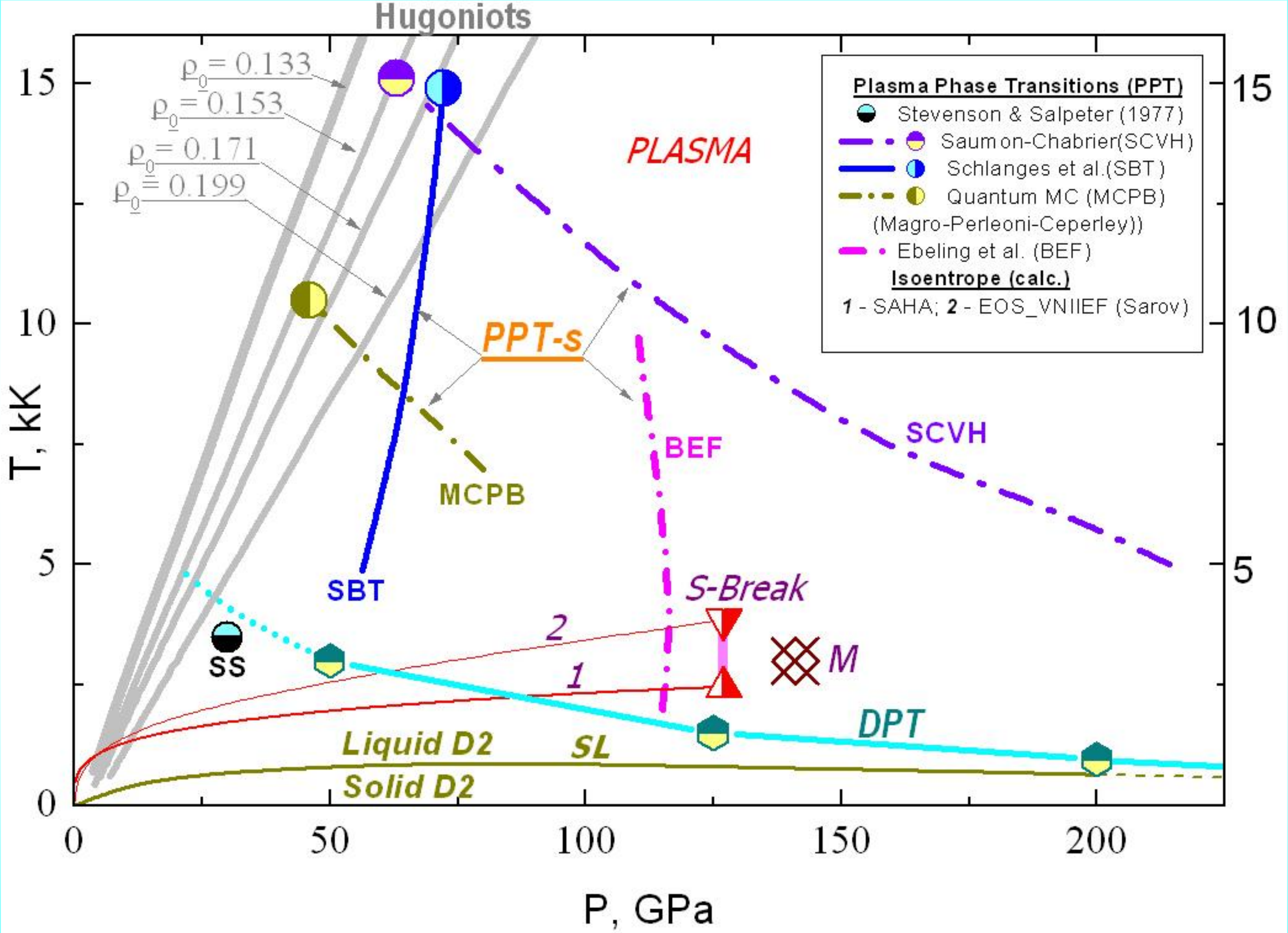
Figure from:
C. Toepffer et al,
"Physics of High Energy Density in Matter"
(2007)

Friedrich-Alexander-Universität Erlangen-Nürnberg

Wave Packet Molecular Dynamics (WPMD) Theory (2007)

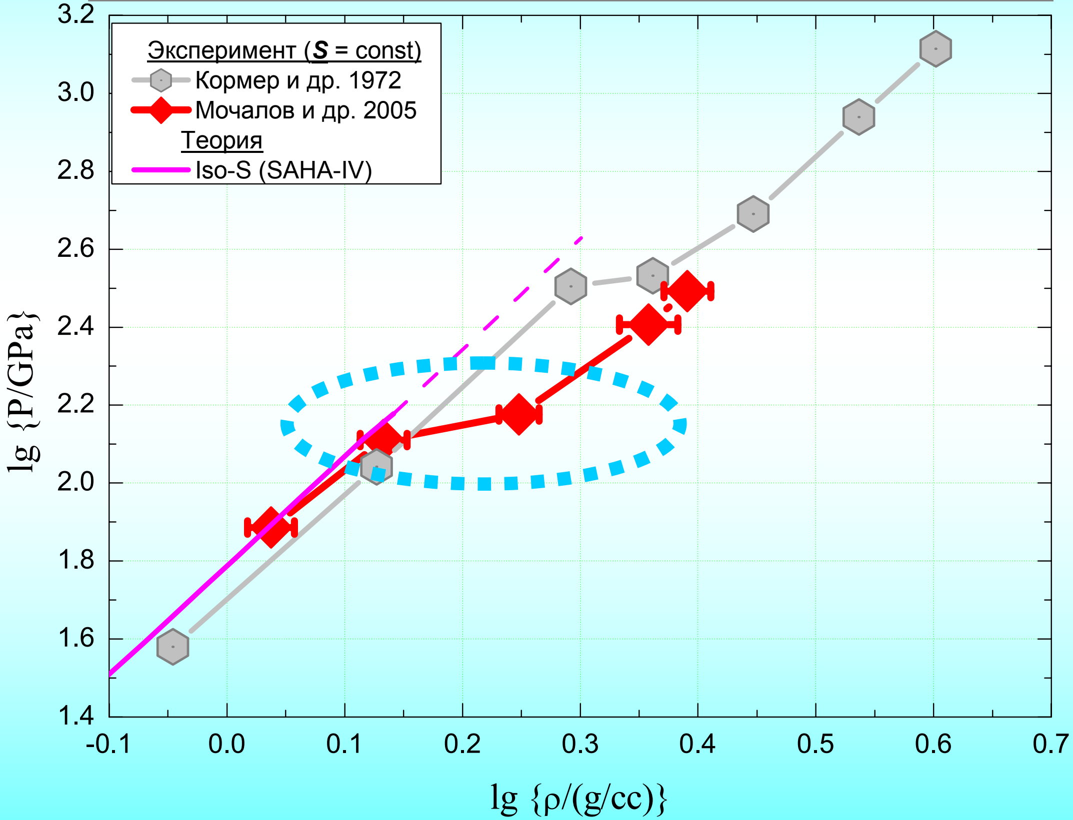
[*] **Jakob B**. *Doctoral Thesis, Erlangen University* (2006) // Submitted to ***PRE*** (2007)

Problem of experimental confirmation of theoretically predicted phase transitions in hydrogen



Quasi-isoentropic compression gaseous deuterium up to the pressure 75-300 GPa

Density “jump” at isentropic compression

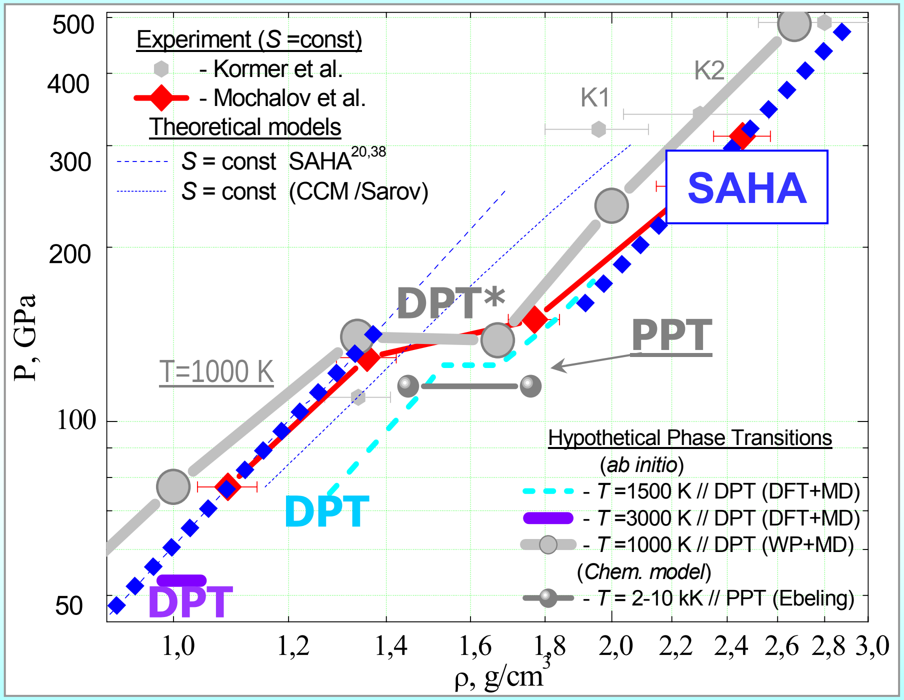


After:
M. Mochalov *et al.*
SCCS-2005,
Moscow

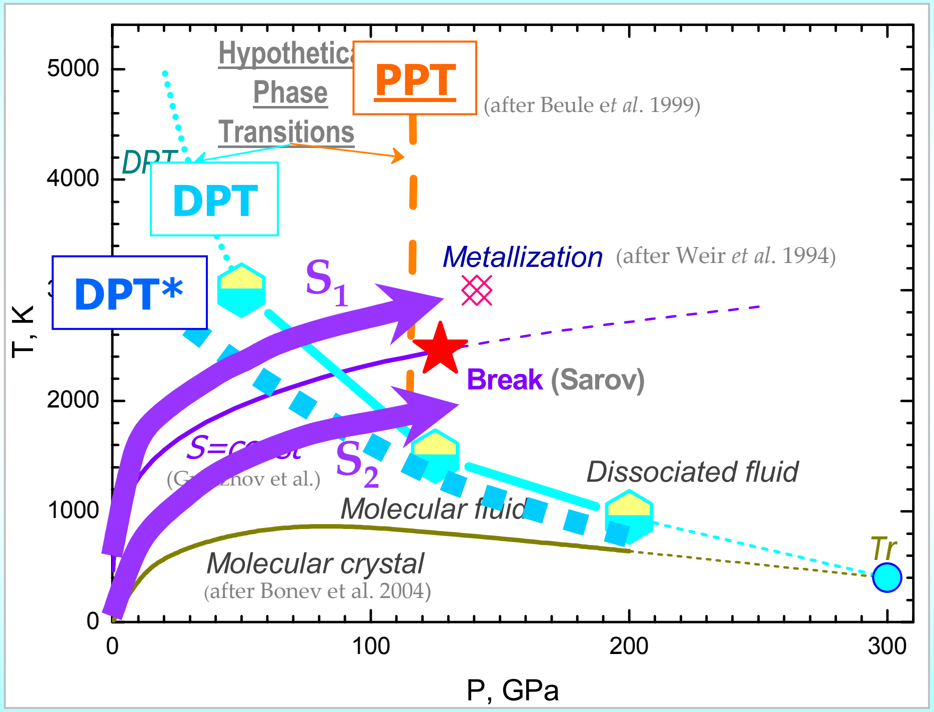
SAHA-IV: - Chemical model (Gryaznov et al.) with modified Coulomb corrections and interaction parameters H_2-H_2 / H_2-H / H-H – in accordance with “atom-atomic” approximation (E. Yakub – *Physica* B **265** 31 (1999)

Density break in isentropic compression of gaseous deuterium ⇔ hypothetical phase transition (?)

Pressure-Density Diagram



Pressure-Temperature Diagram



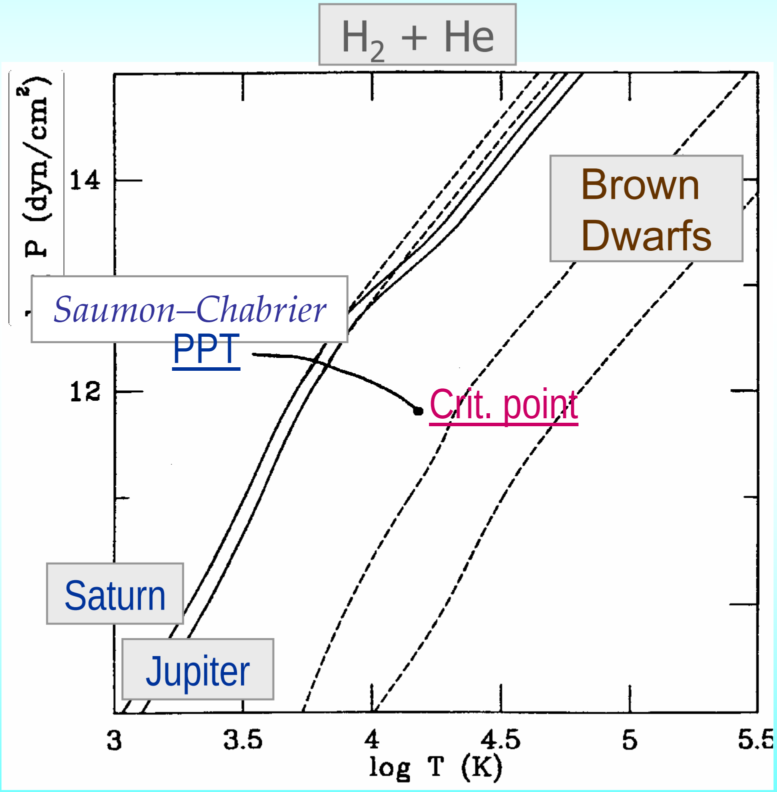
PPT – "Ionization driven" phase transition (Beule D., Ebeling W. et al. *PRB*, 1999)

DPT – "Dissociation driven" phase transition (Scandolo S. 2003 // Bonev S. Militzer B. Galli G. 2004)

DPT* – "Dissociation driven" phase transition (Ab Initio: WPMD // Jakob *et al.* 2007)

Fortov V., Mochalov M. *et al.* (Submitted to *Phys. Rev. Lett*.) // Iosilevskiy I., Gryaznov V., Fortov V. (to be published)

Hypothetical phase transition in H_2/He mixture ⇔ ⇔ Planets evolution problem (?)



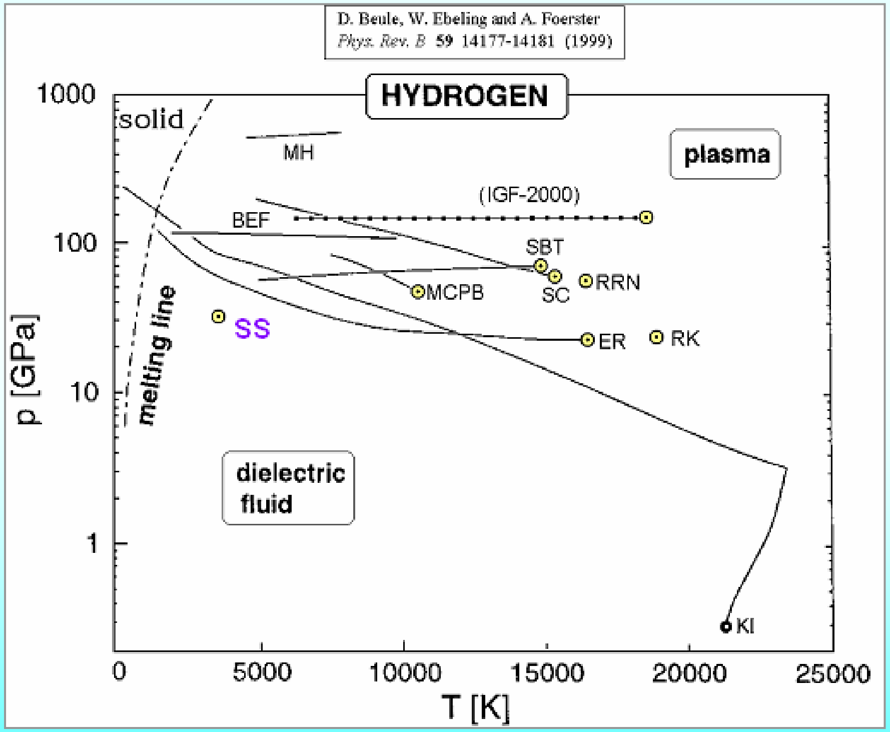
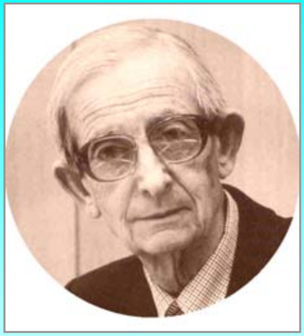


FIG. 3.—Adiabats computed from the EOS described in § 2 with a helium mass fraction $Y = 0.24$. The heavy solid line is the coexistence curve of the plasma phase transition and the critical point is indicated by a dot. Solid lines are computed from the EOS with PPT, dashed lines from the interpolated hydrogen EOS (see text). The temperature of the adiabats at the 1 bar pressure level is, from left to right: 135 (Saturn), 165 (Jupiter), 1500, and 3500 K. In a



Int. Conference "Yu. Khariton's Science Readings"

Extreme State of Matter

Russian Federal Nuclear Center, Sarov, March 2001

Non-congruent phase coexistence in uranium-oxygen plasma

Igor Iosilevskiy

Moscow Institute of Physics and Technology (State University)

Victor Gryaznov & Vladimir Fortov

Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia

Eugene Yakub

Odessa State Economic University, Ukraine

Alexander Semenov

Moscow Power Engineering Institute, Russia

Claudio Ronchi

Institute for Transuranium Elements, JRC, Karlsruhe, Germany

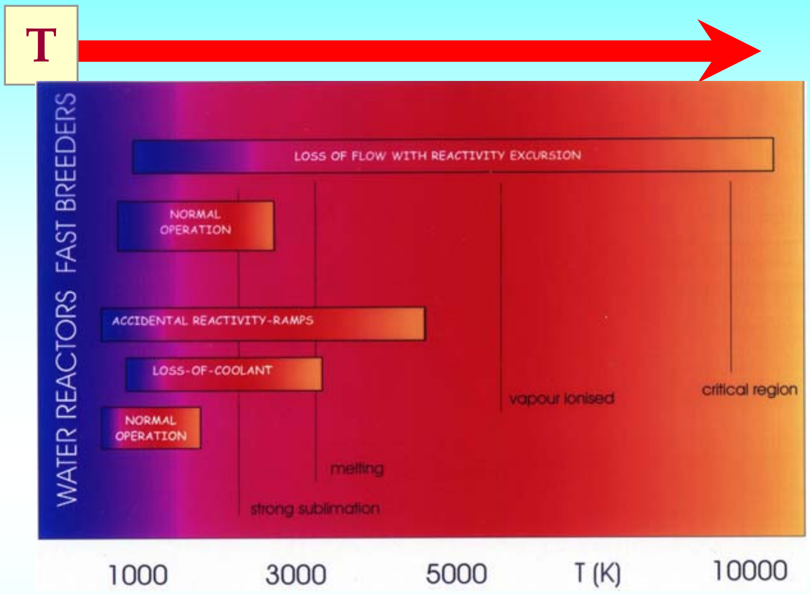
Gerard J. Hyland

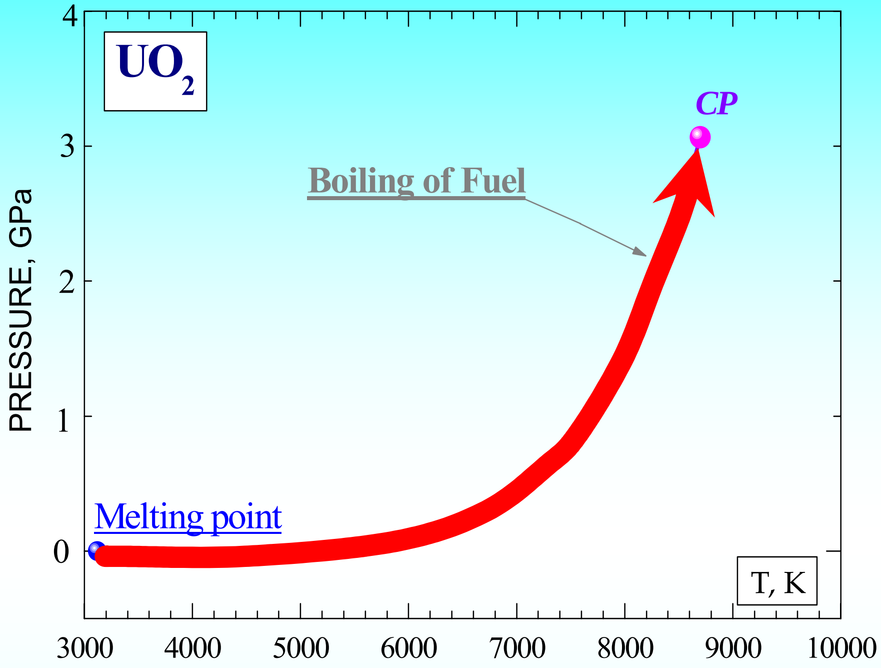
University of Warwick, Coventry, United Kingdom

IPCP RAS — MIPT — JOINT RESEARCH CENTRE Institute for Transuranium Elements — OSEU

Non-Congruent Phase Transition in Uranium Dioxide

Expected Temperature at Hypothetical **Severe Accident** at Fast-Breeder **Nuclear Reactor**





INTAS Project (1995–2002)

Cooperation: **MIPT – IHED RAS – IPCP RAS – OSEU – MPEI** ⇔ **ITU** (JRC, Germany)

Project Coordinator – C. Ronchi (ITU, JRC) ⇔ Project Supervisor – V. Fortov

ISTC Project (2002–2005)

Cooperation: **MIPT – IHED RAS – IPCP RAS – ITEP – VNIIEF** ⇔ **GSI** (JRC, Germany)

Project Manager – B. Sharkov (ITEP, Moscow) ⇔ Project Science Supervisor – V. Fortov

VNIIEF Russian Federal Nuclear Center · IHED RAS · JOINT RESEARCH CENTRE Institute for Transuranium Elements · itu · GSI Gesellschaft für Schwerionenforschung · MIPT · IPCP RAS · OSEU · ITEP (Moscow)

Sketch of theoretical approach

Quasi-chemical representation for liquid & gaseous phases

Ionic Model (*Liquid*)	Multi-molecular Model (*Liquid & Gas*)
$U^{6+} + U^{5+} + U^{4+} + U^{3+} + O^{2-} + O^{-}$	$U + O + O_2 + UO + UO_2 + UO_3$ $U^{+} + UO^{+} + UO_2^{+} + O^{-} + UO_3^{-} + e^{-}$

Interactions: (*Pseudopotential components*)

- Intensive Short-range Repulsion
- Coulomb Interaction between Charged Particles
- Short-range Effective Attraction between all Particles

Interaction corrections: (*Modified for mixtures*)

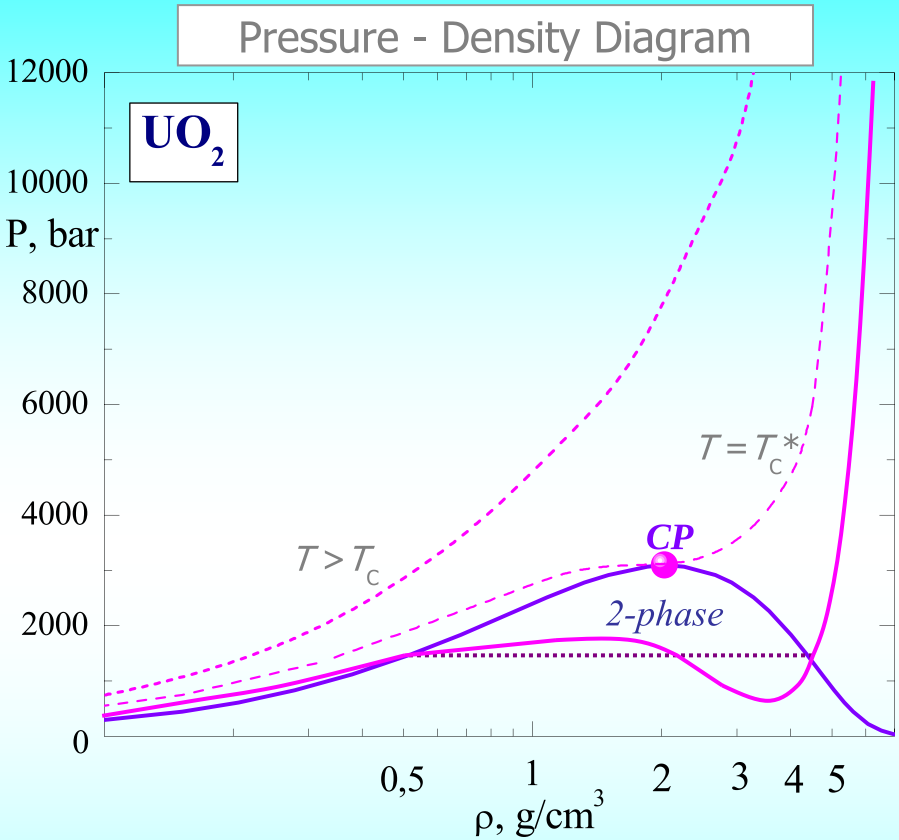
- Hard-sphere Mixture with Varying Diameters
- Modified Mean Spherical Approximation (MSAE+DHSE)
- Modified Thermodynamic Perturbation Theory {TPT- $\sigma(T)$; $\varepsilon(T)$}

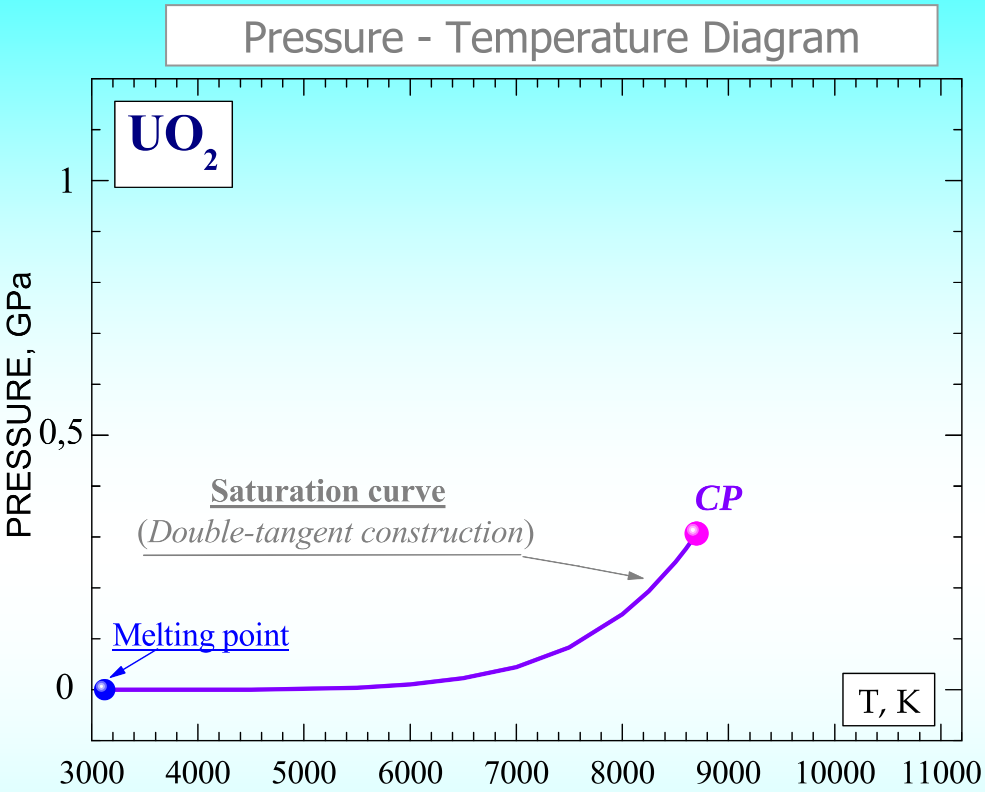
* Iosilevskiy I., Yakub E., Hyland G., Ronchi C. *Int. Journal of Thermophysics* **22** 1253 **(2001),**

* Iosilevskiy I., Gryaznov V., Yakub E., Ronchi C., Fortov V. *Contrib. Plasma Phys*. **43**, N 5-6 316 (**2003**)

* Ronchi C., Iosilevskiy I., Yakub E., *Equation of State of Uranium Dioxide* / **Springer, Berlin,** (**2004**)

Forced-congruent evaporation in U-O system





- Stoichiometry of coexisting phases are equal: $x' = x''$ $\quad$ $x' \neq x''$
- Van der Waals loops (at $T < T_c$) corrected via the "double tangent construction"
- Standard phase equilibrium conditions:

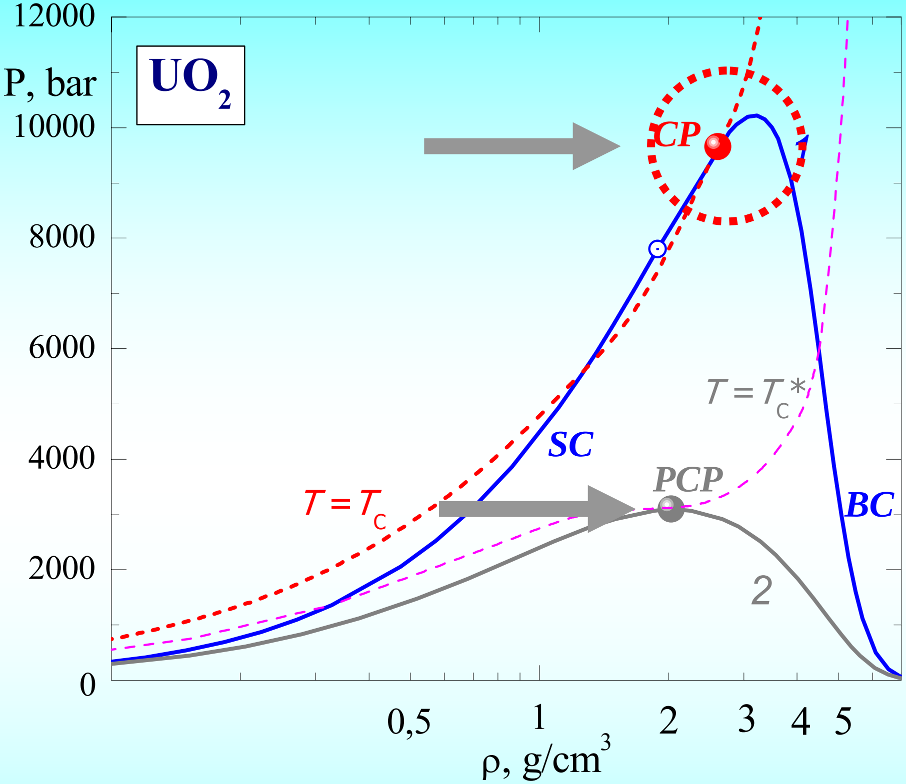
$$P' = P'' \quad // \quad T' = T'' \quad // \quad G'(P,T,x) = G''(P,T,x) \quad \mu_i'(P,T,x') = \mu_i''(P,T,x'')$$

- Standard critical point:

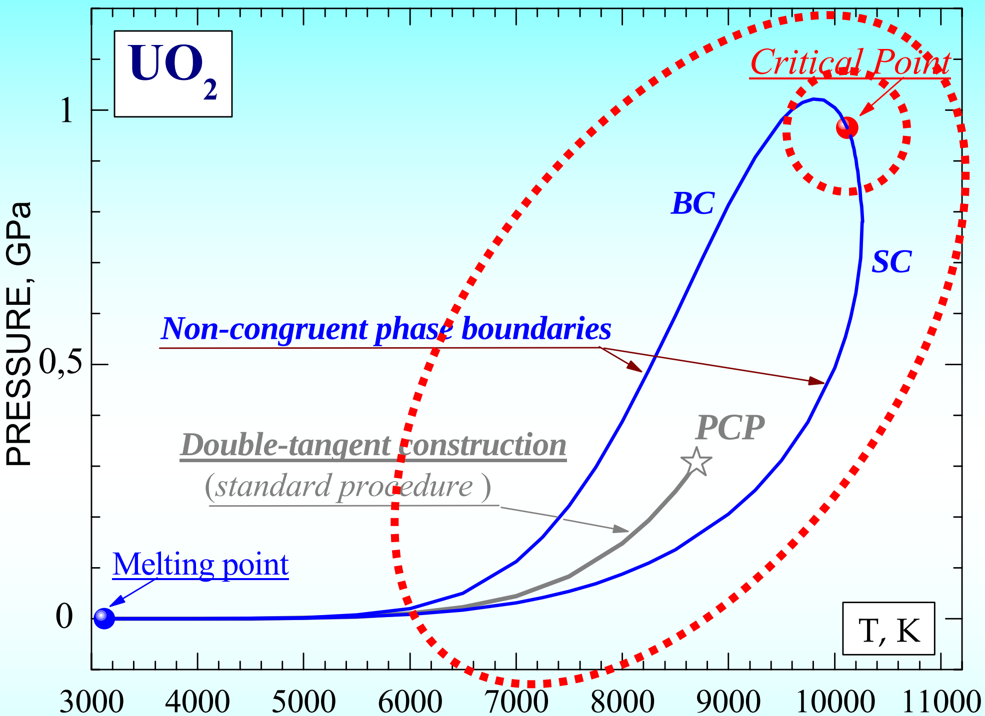
$$(\partial P/\partial V)_T = 0 \quad // \quad (\partial^2 P/\partial V^2)_T = 0 \quad // \quad (\partial^3 P/\partial V^3)_T < 0$$

Non-congruent evaporation in U-O system

Pressure - Density Diagram



Pressure - Temperature Diagram



1 – Non-congruent (total) equilibrium

2 – Forced-congruent (partial) equilibrium

BC – Boiling (liquid) conditions

SC – Saturated (vapor) conditions

NB! **2-dimensional** two-phase **region** instead of standard *P-T* **saturation curve**

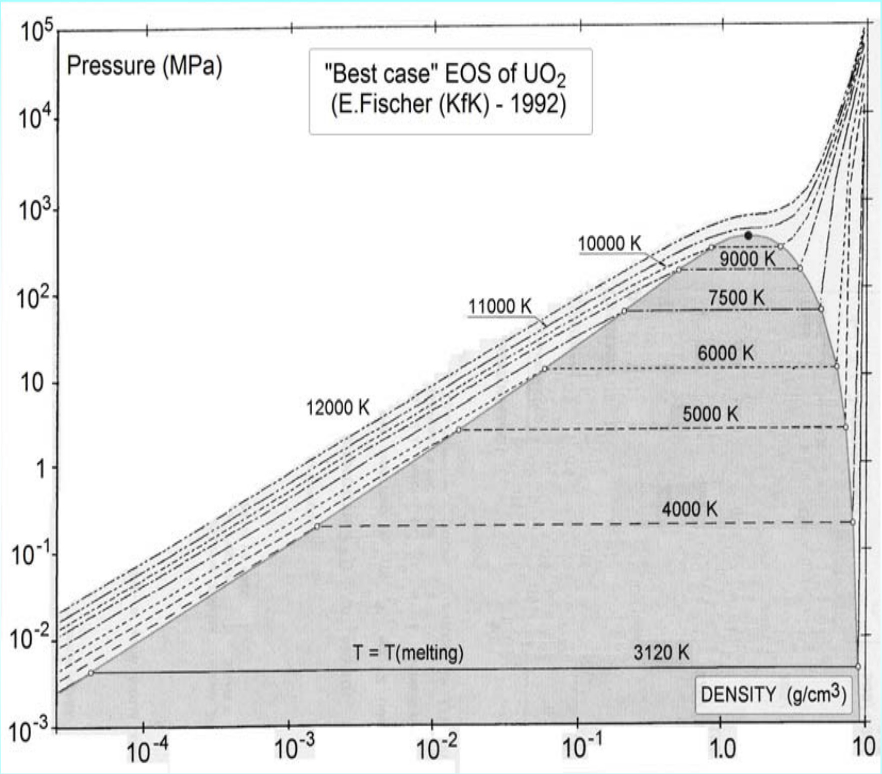
NB! **High pressure level** of non-congruent phase decomposition

NB! **Critical point** should be of **non-standard** type: $(\partial P/\partial V)_T \neq 0$ $(\partial^2 P/\partial V^2)_T \neq 0$

It should be instead: $(O/U)_{liquid} = (O/U)_{vapor}$ $\|\partial\mu_i/\partial n_k\|_T\}_{cp} = 0$

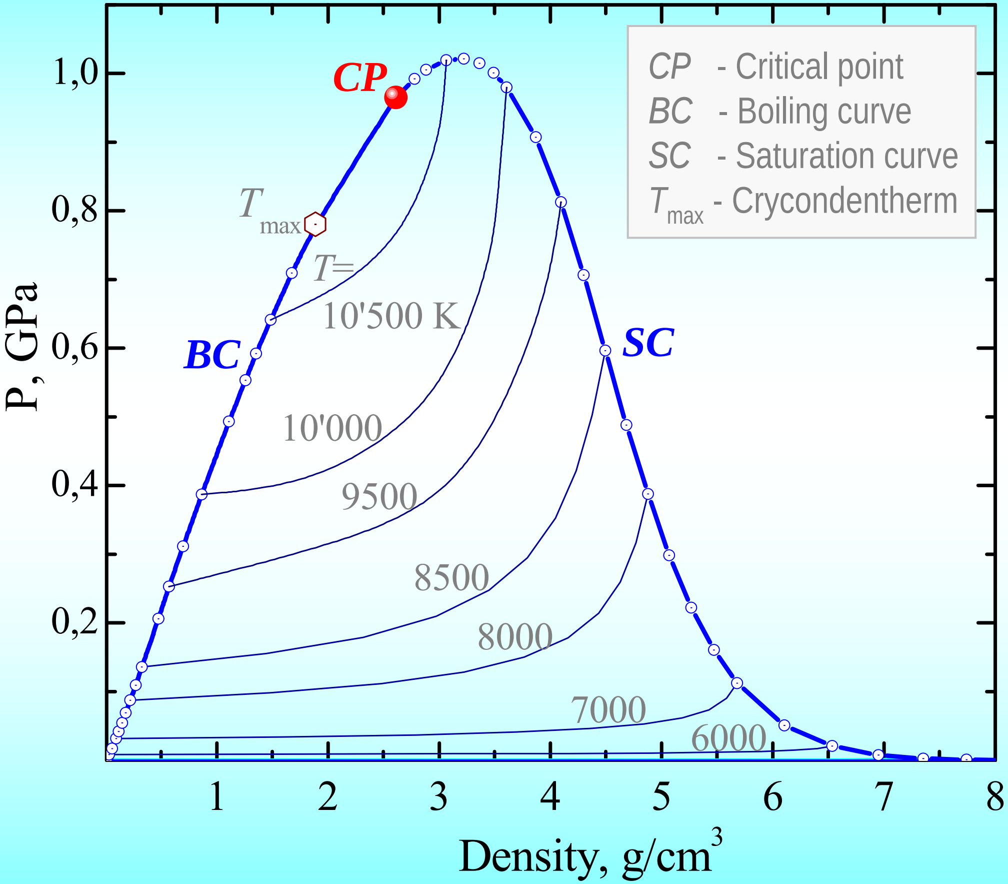
Isotherms in Two-Phase Region

Standard pressure-density diagram



Fischer E.A. *Journal of Nuclear Science and Engineering*. **101** 97 (1989)

Non-congruent phase transition

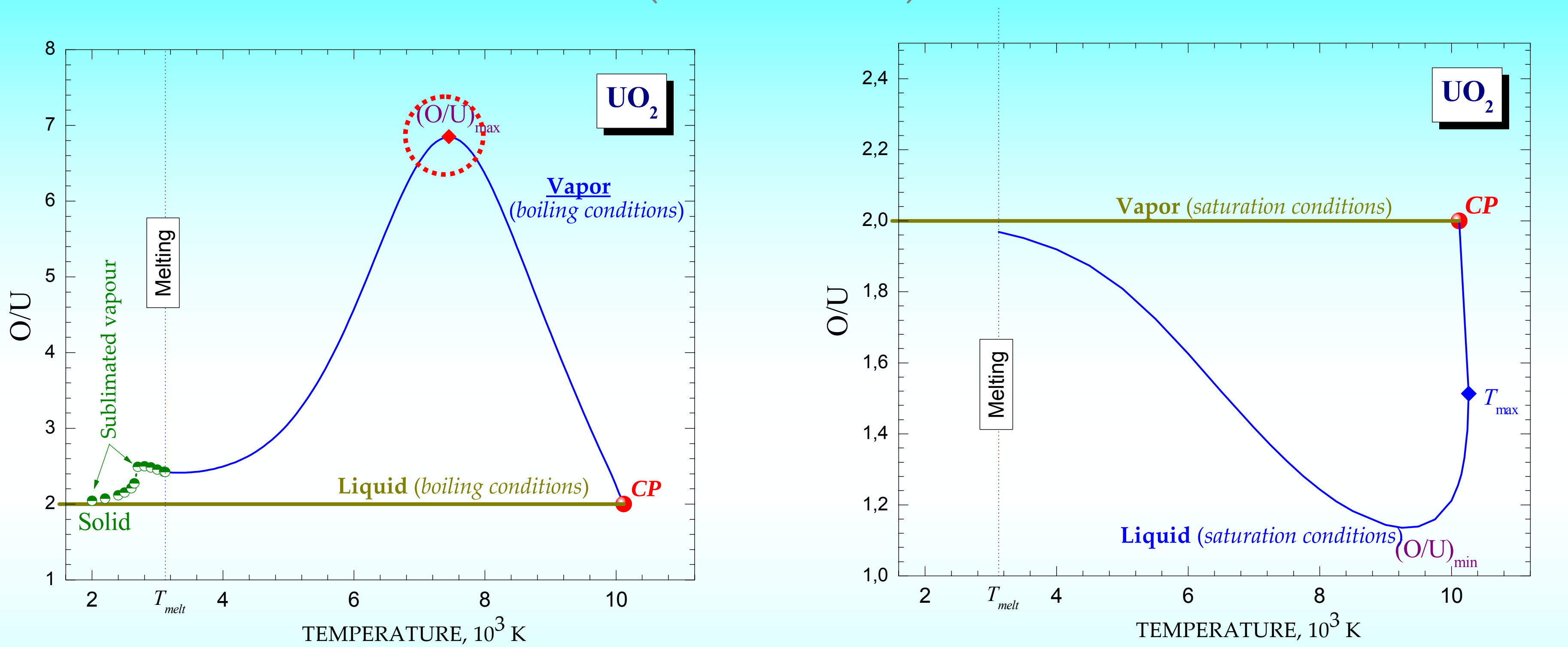


- **Isothermal** phase transition starts and finishes at ***different pressures***
- **Isobaric** phase transition starts and finishes at ***different temperatures***

Non-congruent evaporation in U – O system

Stoichiometry of Coexisting Phases

(two limits)



Boiling Conditions	Saturation Conditions
Liquid (O/U = 2.0) ⇔ Vapor (O/U > 2.0)	Vapor (O/U = 2.0) ⇔ Liquid (O/U < 2.0)
First vapor bubbles over the boiling $UO_{2.0}$ *(oxygen enriched)*	First liquid drops in vapor $UO_{2.0}$ ("dew point")

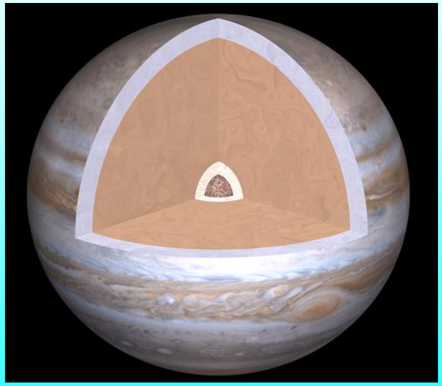
NB! High oxygen enrichment of vapor over the boiling UO(2.0)

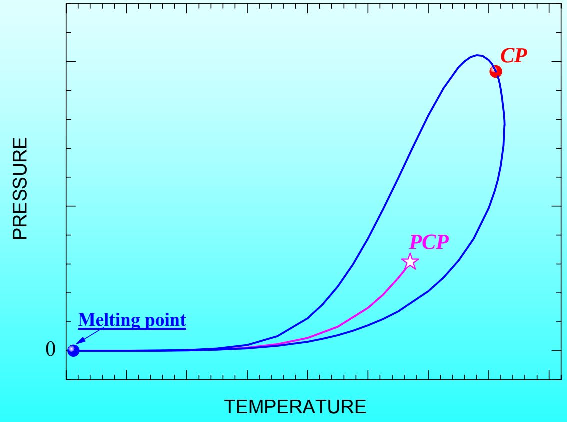
Non-congruence of phase transition in U-O system – – is it an exclusion or a general rule ?

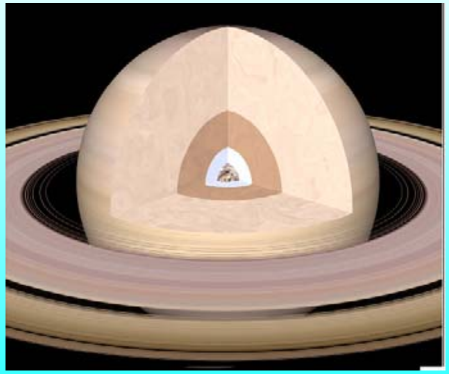
Basic conclusion

- Any phase transition in a system of **two or more chemical elements** must be **non-congruent**.
- Congruent phase transitions are exclusion.

- **Hypothetical example of non-congruent phase transition**
  - *"**Plasma Phase Transition**" (PPT) in H_2/He mixture in **Jupiter, Saturn** (GP), **brown dwarfs** (BD) and **extra-solar giant planets** (EGP) .*



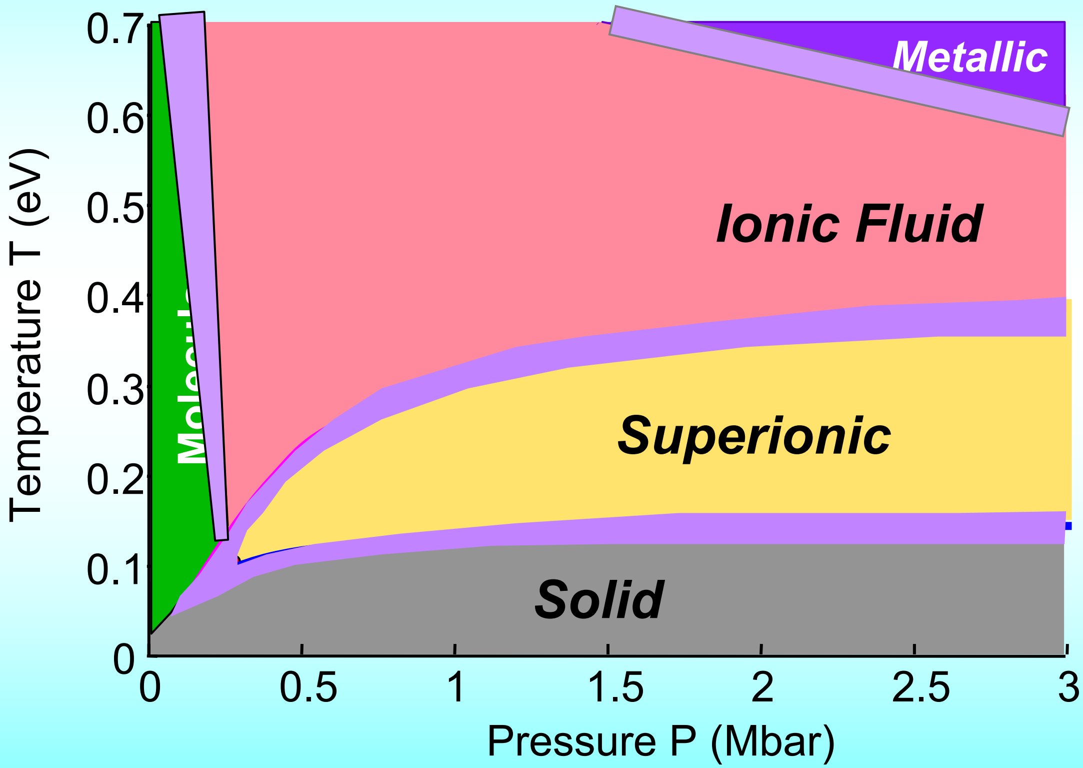




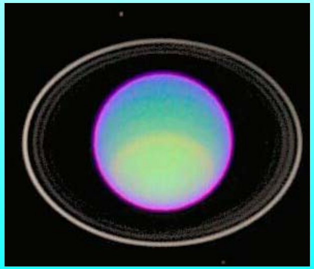
Non-congruent phase transitions in astrophysical objects

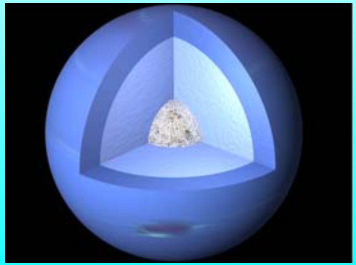
Neptune

Water (Phase Diagram*)



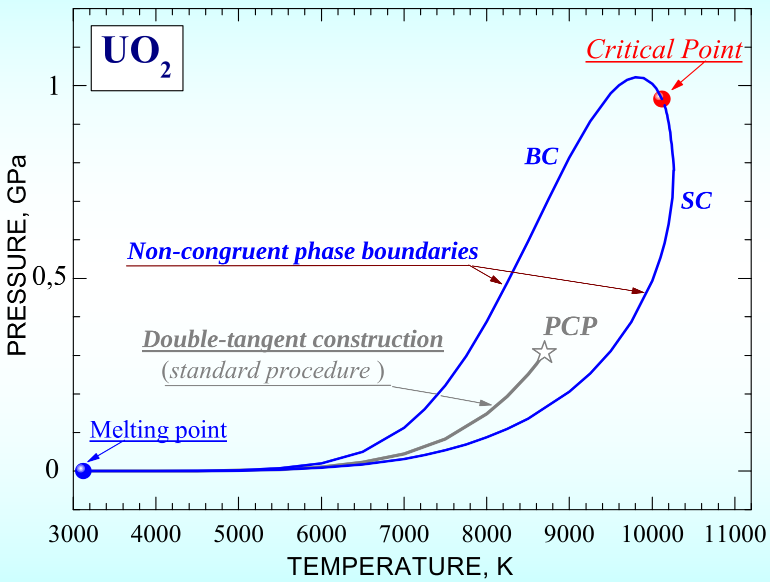
(*) C. Cavazzoni *et al.*, 1999



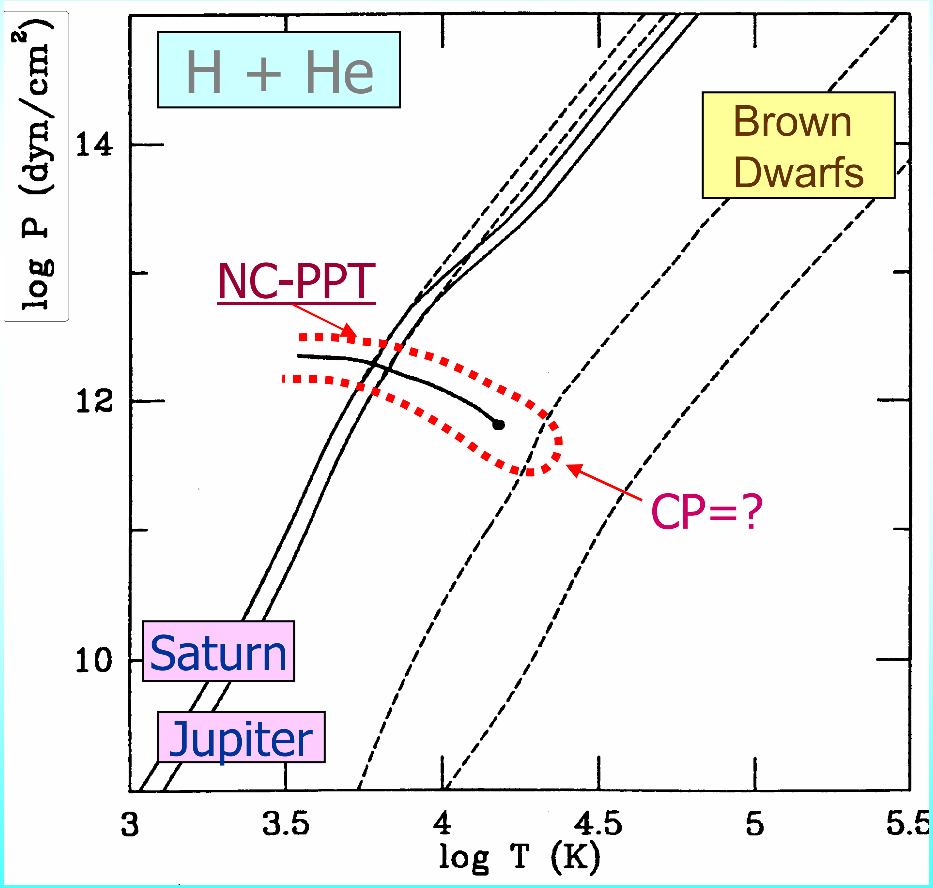


Hypothetical non-congruent plasma phase transition in (H_2 + He) mixture in interiors of Jupiter and Saturn

Non-congruent phase transition in U–O system



Non-congruent PPT in H_2–He system (NC-PPT)



NB!

Two-phase region in H2/He must be non-conventional two-dimensional domain instead of one-dimensional curve

Iosilevskiy I., Gryaznov V., Yakub E., Ronchi C., Fortov V. *Contrib. Plasma Phys.* **43**, N 5-6 316 (2003)

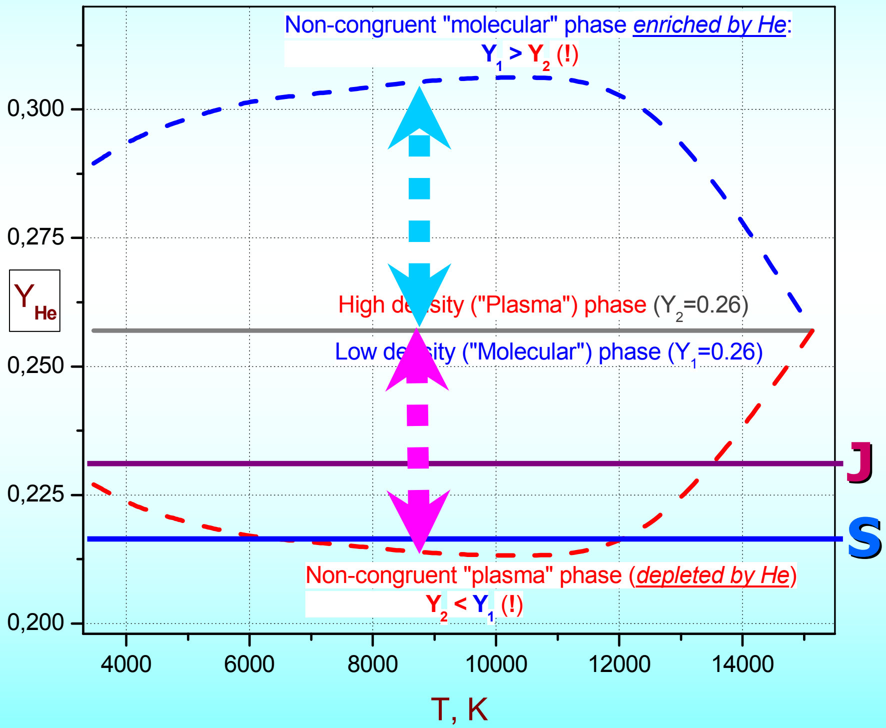
совместно с А.Украинцем (МФТИ)

Estimated non-congruence for plasma phase transition in H_2/He mixture of Jupiter and Saturn

(PPT-variant of Saumon, Chabrier and Van Horn – 1995)

Сб.“Фи
ред. Е

Вопрос:
- Является ли оцененная величина гелиевого обогащения (обеднения) пренебрежимо малой, или же заметной?



Phase Separation in Giant Planets:

Jonathan J. FORTNEY, William B. HUBBARD

Icarus, 164 (1) 2003

Atmospheric elemental abundances in Jupiter and Saturn
(*mass fractions*)

Element	SOLAR	JUPITER *Galileo*	SATURN *Voyager*	SATURN **revised**
H	0.736	0.742	0.92	0.76
He	**0.249**	**0.231** ± 0.04	**0.06** ± 0.05	**0.215** ± 0.035

* Результаты оценки гипотетической неконгруэнтности ПФП в версии Saumon & Chabrier оправдывают ***полномерный расчет*** этого эффекта.

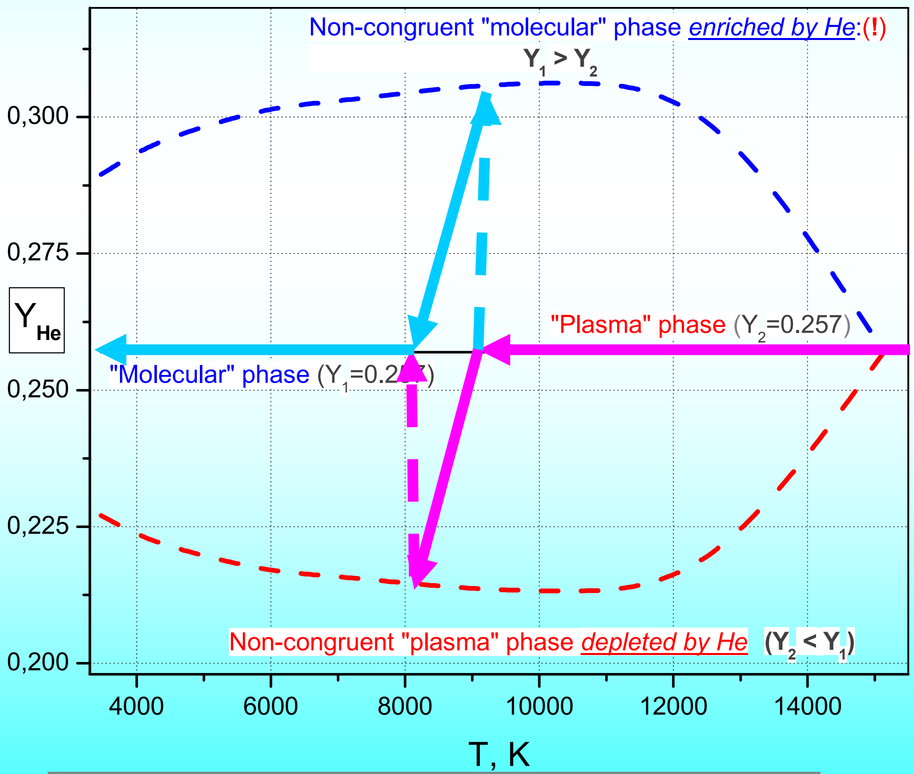
- Это справедливо для ***всех вариантов*** гипотетических фазовых переходов, предсказываемых в чистом водороде и гелии, когда эти ФП переносятся в смесь H_2/He.

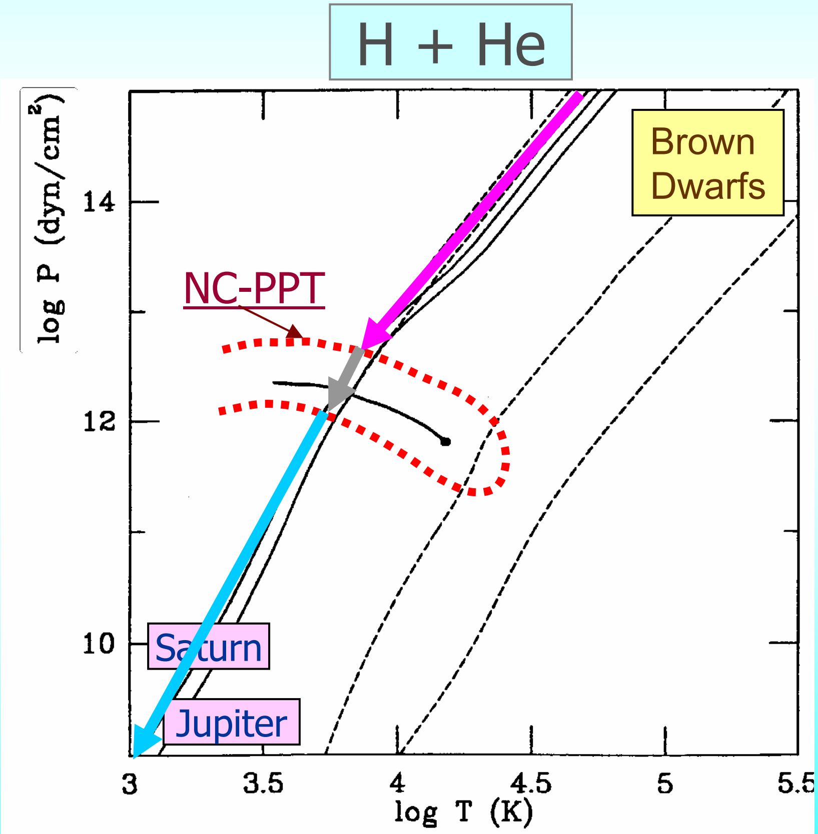
Estimated non-congruence for plasma phase transition in H_2/He mixture of Jupiter and Saturn

(*PPT-variant of Saumon, Chabrier and Van Horn – 1995*)

Assumptions:

- Helium is not ionized.
- Atomic helium interacts with neutral hydrogen species only (H_2 and H).
- Interaction of atomic helium with charged species are low and repulsive.





A. Ukrainets & I. Iosilevskiy
in "*Physics of matter under extreme conditions*",
Ed. V.Fortov, Moscow, IPCP (2005) 116. (*in Russ.*)

Assume we know thermodynamics of pure H_2 and He: How could we obtain the thermodynamics of H_2 + He mixture?

"Additivity approximation" is widely used for this purpose:

$$\mathbf{EOS}(H_2 + He) = x_{H2}\mathbf{EOS}(H_2) + (1 - x_{H2})\,\mathbf{EOS}(He)$$

(A-1): **Additivity of specific enthalpies** ($h = H/M$)

$$\boldsymbol{h}_{(A+B)}(P,T) = x_A\,\boldsymbol{h}_{(A)}(P,T) + (1 - x_A)\boldsymbol{h}_{(B)}(P,T)$$

(A-1): **Additivity of specific volumes** ($v = 1/\rho$)

$$\boldsymbol{V}_{(A+B)}(P,T) = x_A\boldsymbol{V}_{(A)}(P,T) + (1 - x_A)\boldsymbol{V}_{(B)}(P,T)$$

Main issue for the phase transition problem

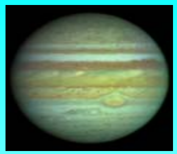
$$(\partial V_{(A)}/\partial P)_T = \infty \quad \longrightarrow \quad (\partial V_{(A+B)}/\partial P)_T = \infty$$

Critical point(s) and **(*P,T*)-coexistence curve(s)** of PT(s) in H_2/He mixture **are the same** identically as those of phase transition(s) in pure H_2 and He

Conclusion:

P-T phase diagram of H_2/He mixture in frames of "**additivity approximation**" is **superposition** of P-T phase diagrams of pure hydrogen and helium.

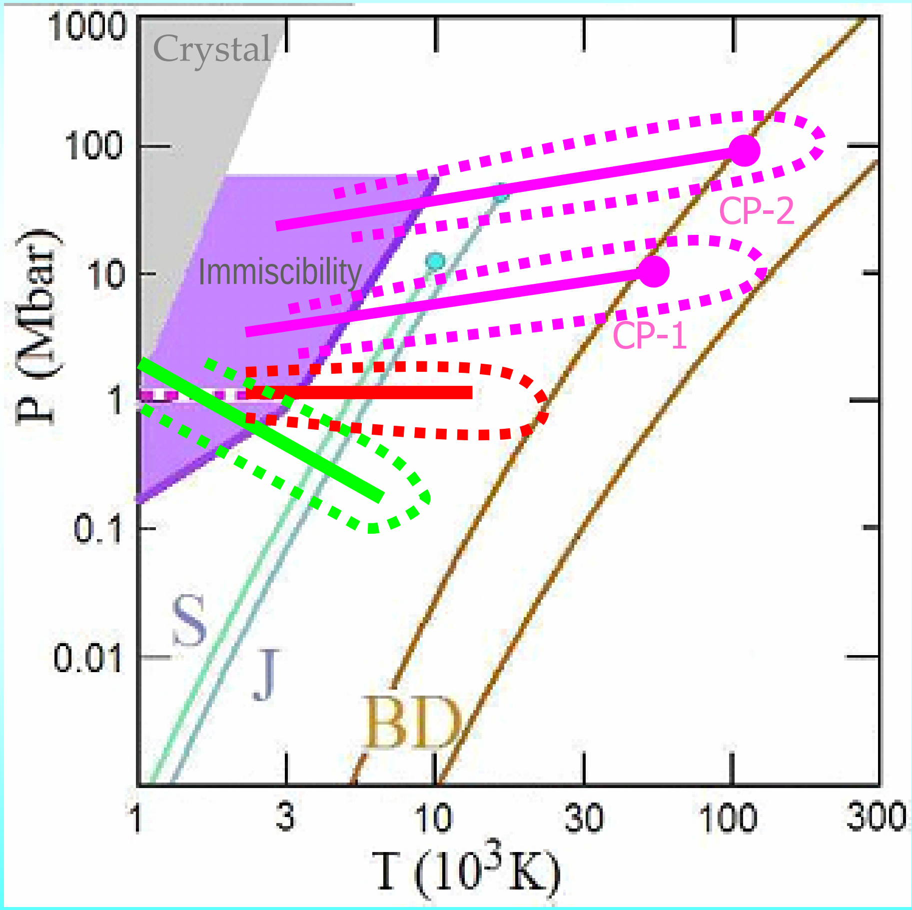
Hypothetical phase transitions in interiors of GP-s and BD-s via "additivity approximation"



(optimistic)

Phase diagram of H_2/He mixture in frames of 'additivity approximation' is **superposition** of *P-T* phase diagrams for pure hydrogen and helium.

H_2 + He



Dissociative Phase Transition in H_2
(*Scandolo S., Bonev S., Militzer B., Galli G.*)

Plasma Phase Transition in **H**
(Ebeling et al.)

1st Plasma Phase Transition in **He**
(Ebeling et al.)

2nd Plasma Phase Transition in **He**
(Ebeling et al.)

Presence of helium relax phase transition in hydrogen **<>** presence of hydrogen relax phase transition in helium

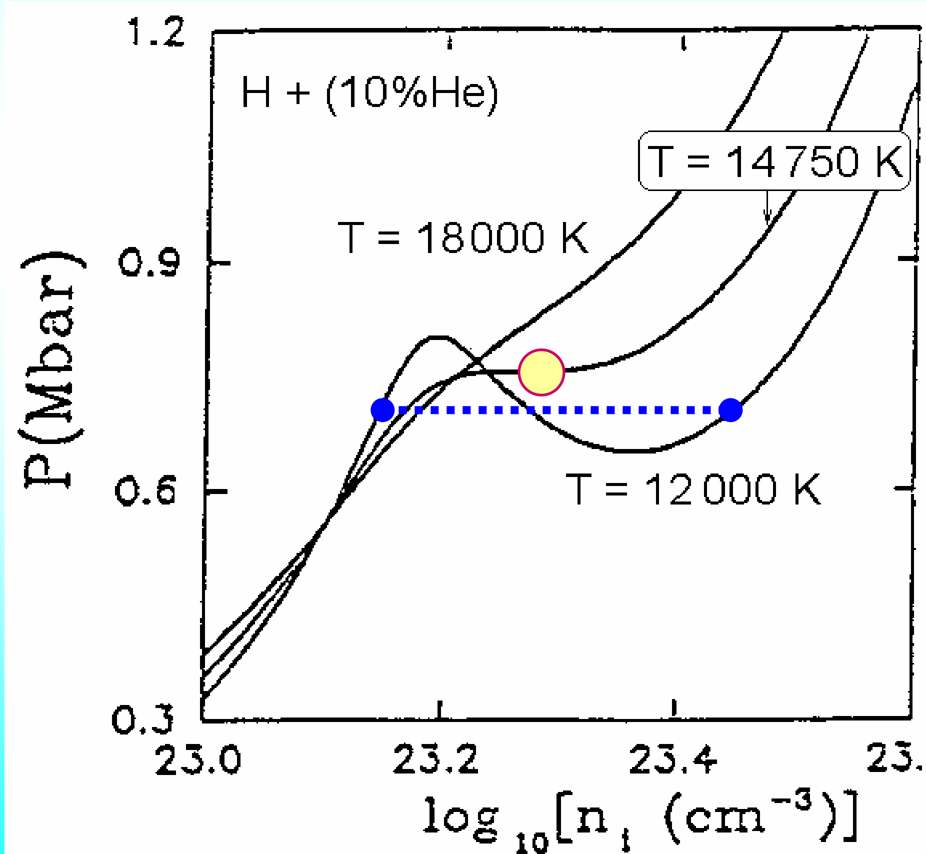
Schlanges M., Bonitz M, Tschetschjan A. *Contrib. Plasma Phys.* **35** 109 (1995)

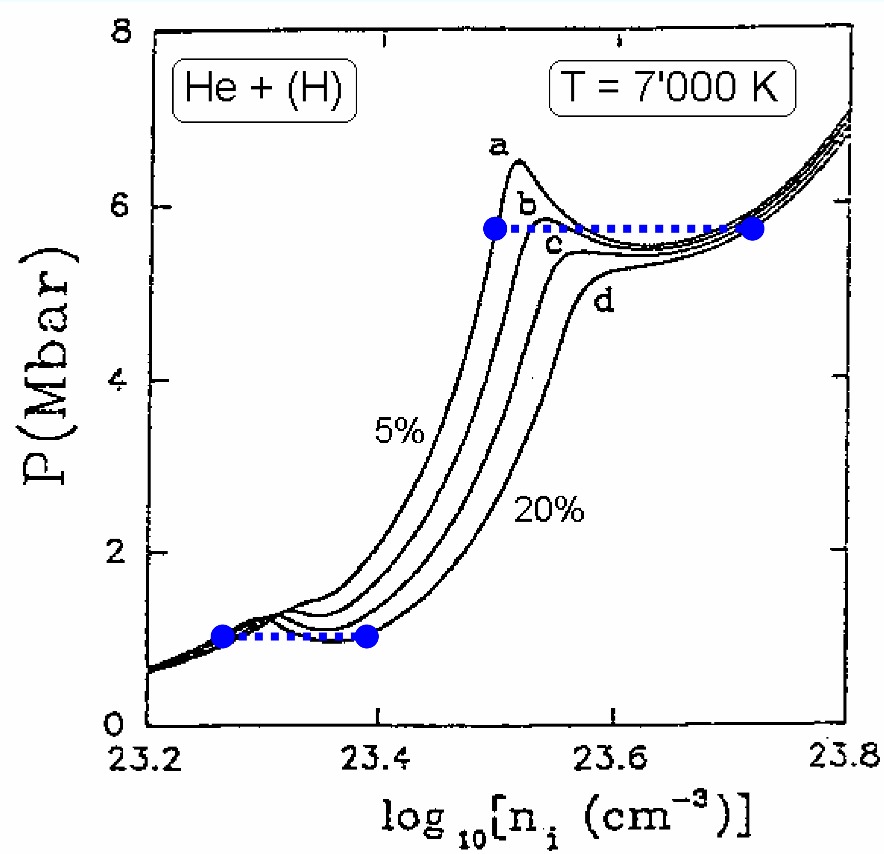
Thermodynamics of H_2 + He plasma

Contrib. Plasma Phys. **35** (1995) 2, 109 – 125

Plasma Phase Transition
in Fluid Hydrogen-Helium Mixtures

M. Schlanges (a), M. Bonitz (b), and A. Tschttschjan (b)





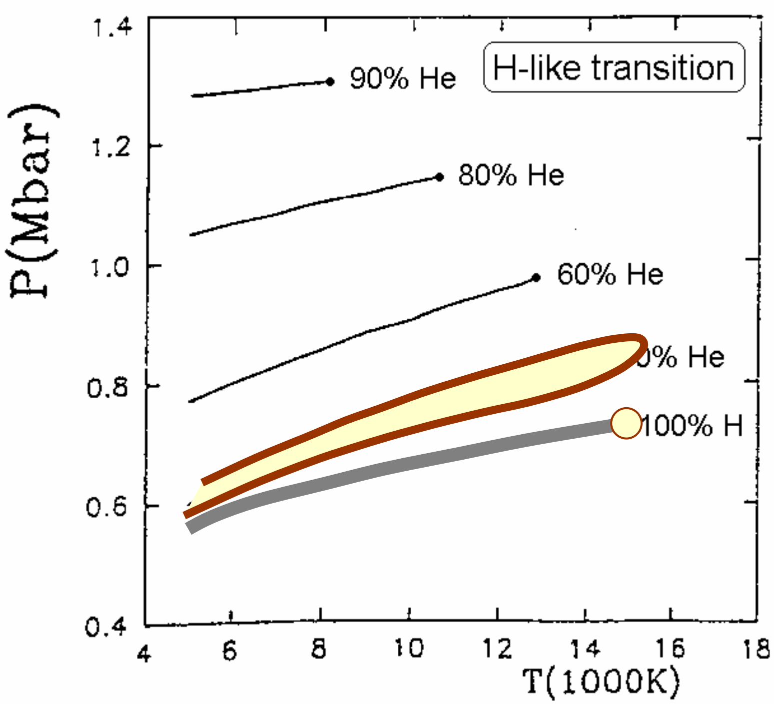
Thermodynamics of $(H_2 + He)$ plasma

(continued)

Contrib. Plasma Phys. **35** (1995) 2, 109 – 125

Plasma Phase Transition
in Fluid Hydrogen-Helium Mixtures

M. SCHLANGES (a), M. BONITZ (b), and A. TSCHTTSCHJAN (b)



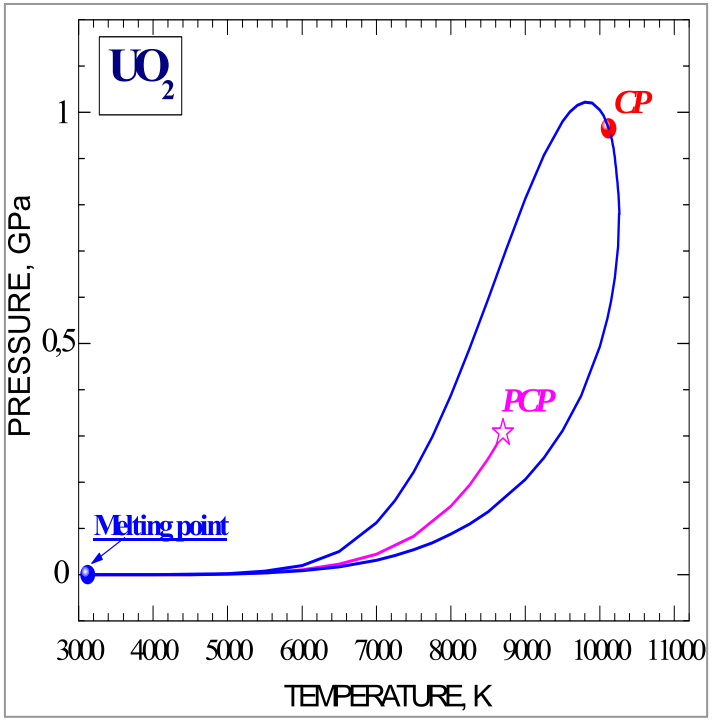


Fig. 7. Coexistence pressure for H – He mixtures for different values of the mixing parameter, for the hydrogen-like plasma phase transition and for the helium-like plasma phase transition.

Elemental Abundance in Solar and Extrasolar Planets

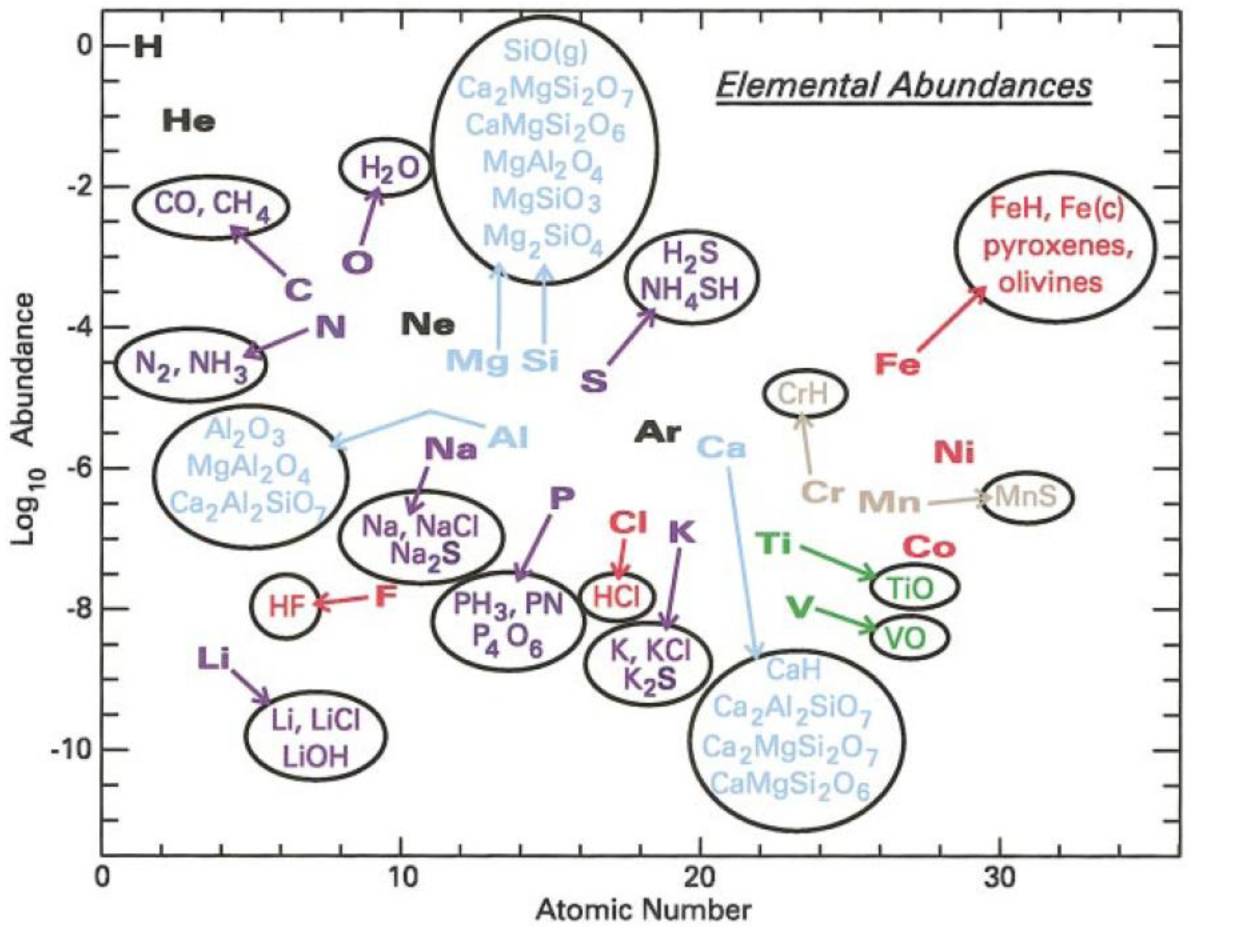


FIG. 10. A plot of the abundance of the elements vs atomic number. The position of the element name indicates its elemental abundance according to Anders and Grevesse (1989); see Table II. The balloons contain representative associated molecules/atoms/condensates of importance in brown dwarf and giant planet atmospheres. See Sec. V in text for discussion [Color].

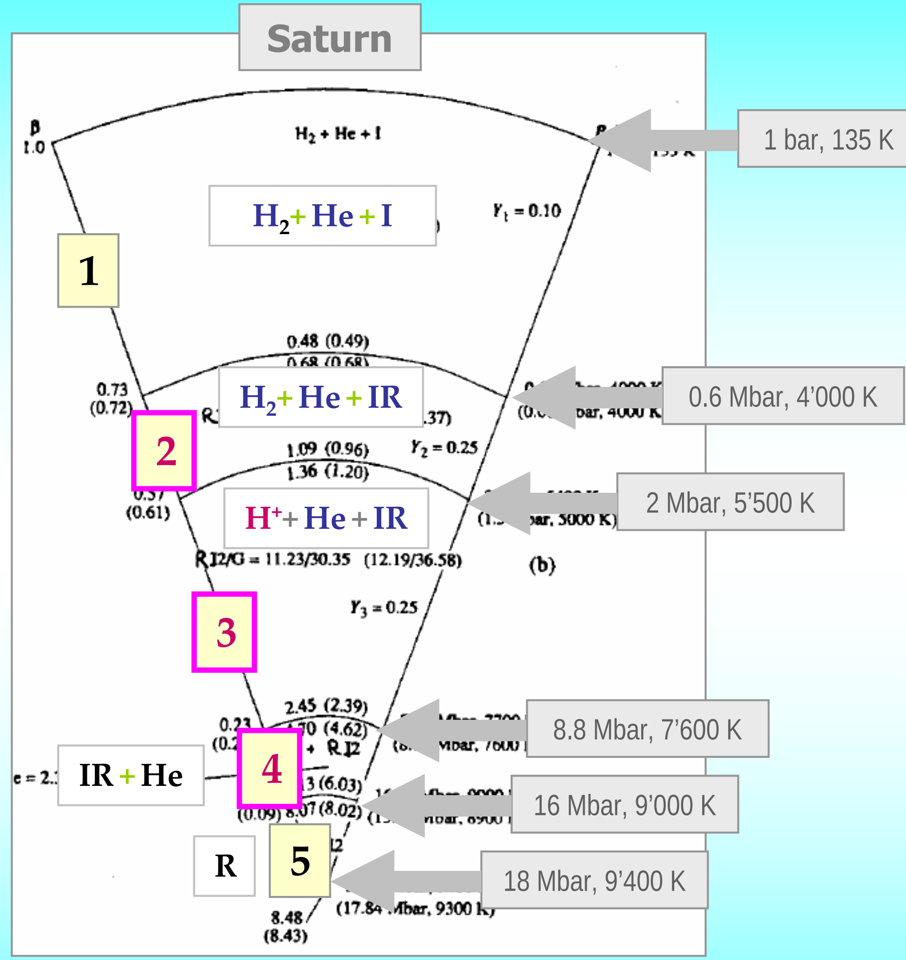
Burrows A., Hubbard W.B., Lunine J.L. and Liebert J. *Rev. Mod. Phys.* **73** 719-769 (2001) *The theory of brown dwarfs and extrasolar giant planets*

Parameters of the Models of Saturn

Table 4
Parameters of the models of Saturn

Model	Y_0	Y_3	Z_{2-4}	P_m	P_{1-2}	M_{He}, core	M_{core}
$Y_1=0.06,\ Y_2=0.25,\ Z_1=0.02,\ I/R=2.2$							
MS1	0.267	0.00	0.30	3.0	0.42	10.66	16.18
MS2	0.171	0.00	0.40	3.0	0.64	4.58	8.59
MS3	0.225	0.00	0.30	2.0	0.44	9.88	15.06
MS4	0.133	0.00	0.40	2.0	0.67	4.02	7.65
MS5	0.274	0.25	0.30	3.0	0.46	6.33	9.99
MS6	0.187	0.25	0.40	3.0	0.72	0.05	1.03
MS7	0.285	0.25	0.25	2.0	0.43	7.34	10.74
MS8	0.244	0.25	0.30	2.0	0.55	4.05	6.74
MS9	0.322	0.35	0.25	3.0	0.36	7.66	11.16
MS10	0.278	0.35	0.30	3.0	0.49	3.80	6.38
MS11	0.237	0.35	0.35	3.0	0.62	0.41	1.58
MS12	0.293	0.35	0.25	2.0	0.48	3.90	6.15
MS13	0.255	0.35	0.30	2.0	0.62	0.81	2.11
MS14	0.282	0.35	0.25	1.5	0.60	2.60	4.42
MS15	0.249	0.35	0.30	1.5	0.75	0.007	0.76
$Y_1=0.10,\ Y_2=0.25,\ Z_1=0.02,\ I/R=2.2$							
MS16	0.275	0.00	0.30	3.0	0.48	10.91	16.54
MS17	0.186	0.00	0.40	3.0	0.73	4.98	9.25
MS18	0.234	0.00	0.30	2.0	0.52	10.22	15.55
MS19	0.149	0.00	0.40	2.0	0.77	4.50	8.45
MS20	0.282	0.25	0.30	3.0	0.53	6.69	10.51
MS21	0.202	0.25	0.40	3.0	0.82	0.57	1.9
MS22	0.277	00.25	0.27	2.0	0.56	6.39	9.7
MS23	0.254	0.25	0.30	2.0	0.64	4.49	7.36
MS24	0.277	0.25	0.25	1.5	0.60	6.64	9.8
MS25	0.263	0.25	0.27	1.5	0.66	5.45	8.41
MS26	0.327	0.35	0.25	3.0	0.43	7.93	11.52
MS27	0.287	0.35	0.30	3.0	0.56	4.16	6.89
MS28	0.248	0.35	0.35	3.0	0.71	0.90	2.34
MS29	0.301	0.35	0.25	2.0	0.57	4.39	6.80
MS30	0.266	0.35	0.30	2.0	0.73	1.36	2.89
MS31	0.291	0.35	0.25	1.5	0.71	3.13	5.12
MS32	0.259	0.35	0.30	1.5	0.87	0.48	1.64

T.V. Gudkova, V.N. Zharkov / Planetary and Space Science 47 (1999) 1201–1210



I – "Ices" (H_2O, NH_3, CH_4) **R** – rocks + Fe + Ni

Y – весовая доля гелия

$\mathbf{Z_G}$ – весовая доля {H_2O, NH_3, CH_4 + Fe + Ni}

Optimized models of Jupiter and Saturn

	JUPITER	SATURN
M ($\oplus$)	317.7	95.1
M_c ($\oplus$)	5	1
M_{ice}/M_c	0.50	0.95
P_c (Mbar)	67.4	15.5
T_c (K)	22600	11900
P_{PPT} (Mbar)	1.71	1.93
T_{PPT} (K)	6880	6070
Y_I	0.29	0.25
Y_{II}	0.326	0.73

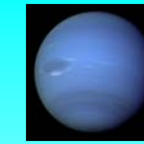
TABLE 1

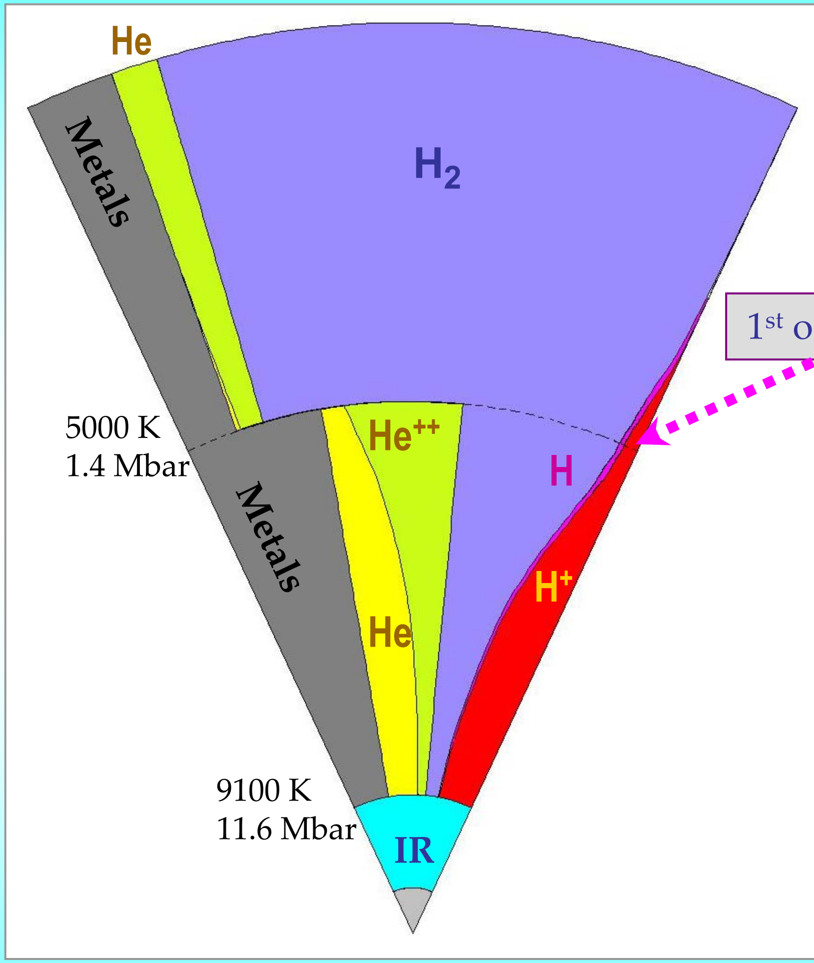
Optimized models of Jupiter and Saturn

GIANT PLANETS AND THE PLASMA PHASE TRANSITION OF HYDROGEN
D. Saumon, G. Chabrier, W. B. Hubbard, and J. I. Lunine 111

Giant planets interior composition

(After N. Nettelmann, R. Redmer, et al., **PNP-12**, Darmstadt, 2006)

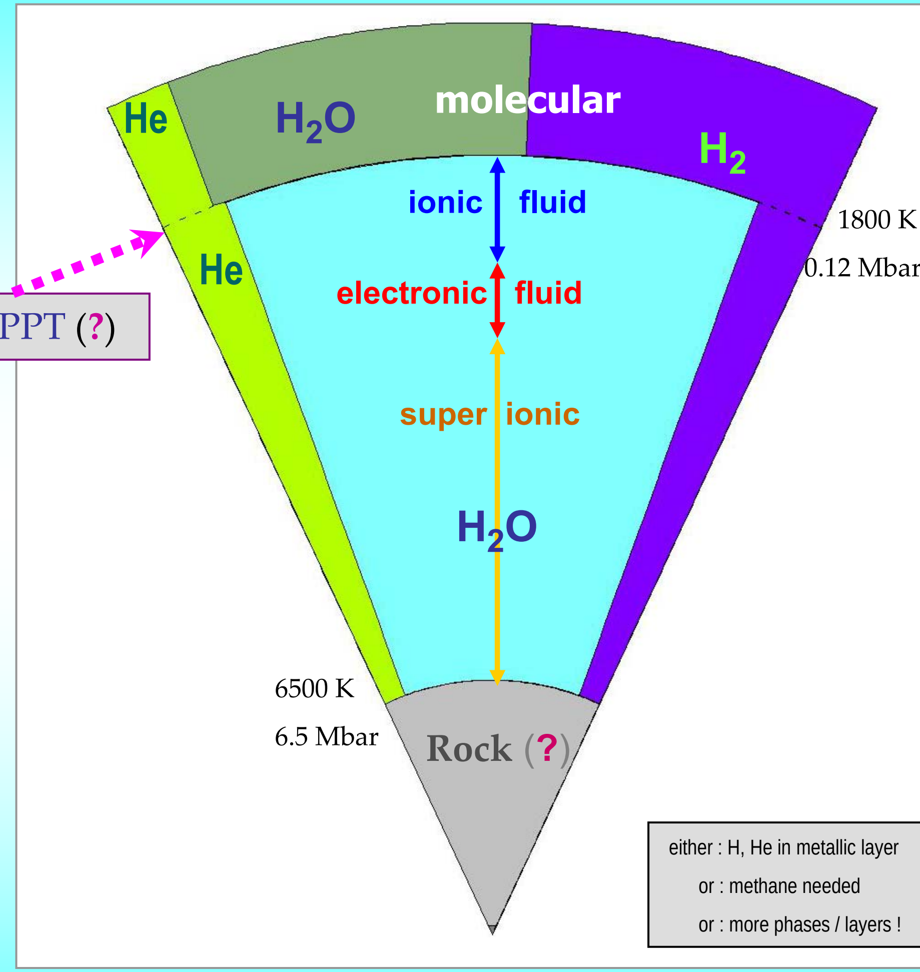




Saturn interior composition using SCVH-95_EOS

(H_2 + He) Saumon, Chabrier & VanHorn (1995)

Ice-Rock core: Hubbard & Marley, *Icarus* **78**, (1989)



Neptune interior composition using Sesame-EOS (G.Kerley,LANL)

(H_2, He, H_2O) EOS from Sesame-EOS-Tables

H_2O phases from DFT-QMD: T. Mattsson

Conclusions and perspectives

- Non-congruence of phase transitions in H_2/He mixture can ‘provoke’ to the H⇔He separation in interiors of *jovian* and *extrasolar* planets and *brown dwarfs*.

- First estimation of non-congruence for SCVH-variant of plasma phase transition in H_2/He mixture approves considering of non-congruence in study of *helium sedimentation* in interiors of Jupiter and Saturn.

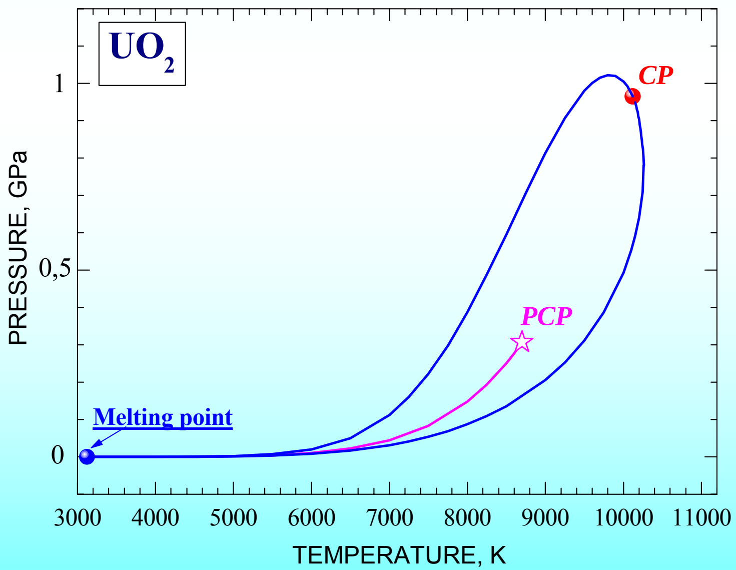
- *Ab initio* approaches are very promising for direct numerical simulation of discussed *non-congruence* for phase transitions in H_2/He mixture in conditions of jovian and extrasolar planets and brown dwarfs.

- New experiments are desirable for study of discussed *non-congruence* for phase transition in H_2/He mixture under conditions of jovian and extrasolar planets and brown dwarfs.

Clearly there will be enough challenges
to keep us all happily occupied for years to come.

Hugh Van Horn (1990)
(Phase Transitions in Dense Astrophysical Plasmas)

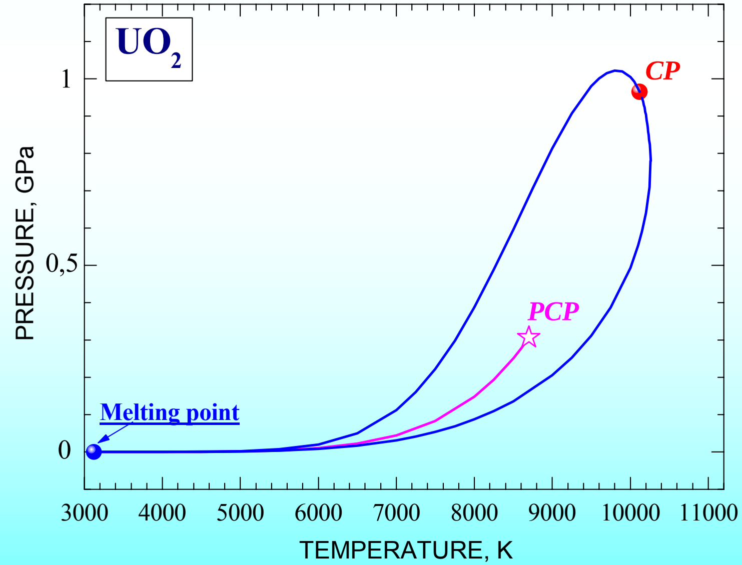
Thank you!



Support: INTAS 93-66 // ISTC 2107 // CRDF № MO-011-0,
and by RAS Scientific Programs
“Physics and Chemistry of Extreme States of Matter” and “Physics of Compressed Matter and Interiors of Planets”

Ioffe Physical-Technical Institute
Department of Theoretical Astrophysics
April 17, 2007

Thank you!



Support: INTAS 93-66 // ISTC 2107 // CRDF № MO-011-0,
and by RAS Scientific Programs
“Physics and Chemistry of Extreme States of Matter” and “Physics of Compressed Matter and Interiors of Planets”