

Seminar for young scientists **Physics of high energy density in matter** <u>FAIR-Russia Research Centre,</u> <u>Moscow, 21-22 November 2011</u>



Non-congruent Phase Transitions *in* **Cosmic Matter** *and* **Laboratory**



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Content

Non-congruence in general The base: Non-congruent phase transition in U-O system Non-congruence in terrestrial and planetary applications Non-congruence in exotic situations (compact stars) Summary

The base

Non-congruent phase transitions in chemically reacting U-O plasma

Non-congruent phase transition in uranium dioxide



INTAS Project (1995–2002)

<u>Cooperation</u>: MIPT – IHED RAS – IPCP RAS – OSEU – MPEI ⇔ ITU (JRC, Germany)

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

ISTC Project (2002–2005)

GSI

Institute for Transuranium Elements

THE

<u>Cooperation</u>: MIPT – IHED RAS – IPCP RAS – ITEP – VNIIEF ⇔ GSI (JRC, Germany)

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

ITEP (Moscow)

Two stages

- Construction of Equation of State (EOS)

- Phase coexistence parameters calculation

Quasi-chemical representation

("Chemical picture")



* I.L.I., Yakub E., Hyland G., Ronchi C. Trans. Amer. Nucl. Soc. 81 (1999) // Int. Journ. Thermophysics 22 (2001)

* I.L.I., Gryaznov V., Yakub E., Ronchi C., Fortov V. Contrib. Plasma Phys. 43, (2003)

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

* I.L.I., Gryaznov V., Semenov A.M., Yakub E., Fortov V. Ronchi C., Hyland G., High Temperature 48, (2010)

* I.L.I., Son E., Fortov V. Thermophysics of non-ideal plasmas. MIPT (2000); FIZMATLIT, (2011)

Quasi-chemical representation

(" Chemical picture" - in plasma community)

Strange (hybrid) stars

<u>U – O system</u>



Two problems in phase transition calculation

- Construction of Equation of State (EOS)

- Phase coexistence parameters calculation



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

P' = P'' || T' = T'' || G'(P,T, x) = G''(P,T, x)

• Standard critical point:

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

Plasma Phase Transitions in H₂ + He plasma

(planetary science)





in Fluid Hydrogen-Helium Mixtures

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





Plasma Phase Transitions in H₂ + He plasma



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.





see for example: Iosilevskiy I., Encyclopedia on low-T plasmas. III-1 (suppl) 2004

Non-congruent evaporation in U-O system (Gibbs - Guggenheim conditions)



Non-congruent evaporation in U – O system

Isotherms in two-phase region



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

Thermodynamics of H₂ + He plasma (planetary science)



Forced-Congruent phase transition in H₂+ He plasma (*calculated*)

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

Plasma Phase Transition

0

in Fluid Hydrogen-Helium Mixtures

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

Non-Congruent phase transition in H₂+ He plasma (*must be instead*!)





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.

Main issue from study of non-congruent evaporation in U–O system

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



Non-congruence in H₂O etc... – what does it mean **?**



<u>BASIC STATEMENT</u>: Any phase transition in a system of two or more chemical elements must be <u>non-congruent</u>



Neptune and "hot-water" extrasolar planets



Any phase transition in *high-T_high-P* water must be *non-congruent*



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<u>BASIC STATEMENT</u>: Any phase transition in a system of **two or more chemical** elements must be <u>non-congruent</u>



Neptune and "hot-water" extrasolar planets



Water (phase diagram - 2011)

R.Redmer, T.Mattsson, N.Nettelman, M.French, Icarus (2011)

Hypothetical phase transitions in H₂/He mixture

Giant planets evolution problem

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

Cassini-Huygens



Fig. 1. Pressure and density profiles of optimized m dens or supiter (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: rock, core, ice market, metallic and molecular

Cassini-Huygens MISSION TO SATURN & TITAN Giant planets evolution problem

Hypothetical phase transitions in H₂/He mixture

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(with Artem Ukrainets)

Estimated non-congruence for plasma phase transition in H₂/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.



Estimated non-congruence for the plasma phase transition in H₂/He mixture of Jupiter and Saturn

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

Question:

- Is the estimated helium enrichment (depletion) negligible or noticeable? (or may be even significant ?)



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 <i>Galileo</i>	SATURN Voyager	SATURN revised
Н	0.736	0.742	0.92	0.76
He	0. 249	$\textbf{0.231} \pm 0.04$	$\textbf{0.06} \pm 0.05$	$\textbf{0.215} \pm 0.035$

- * Provided estimation of the non-congruence for PPT in version of Saumon and Chabrier approves full-size calculation of this effect.
- * The same is true for all other variants of predicted hypothetical phase transitions in pure hydrogen and helium when they being transformed into H2/He mixture.



Giant planets interior composition





Предсказания плазменных фазовых переходов Модельные подходы (1970 – 2007)





Два раздельных плазменных перехода в гелии (на 1^й и 2^й ионизации)

Ebeling, Foerster et al. (1991)

Ландау Л.Д. Зельдович Я.Б. ЖЭТФ 14 32 (1944)

Норман Г.Э., Старостин А.Н. ТВТ (1968 - 1970)

Фазовый переход в плазме водорода уверенно предсказывается различными вариантами первопринципных подходов



DFT + MD / **Bonev**, Militzer, Galli.



DFT + MD / Morales M. et al. (2010)/ Lorenzen W. et al. PRB (2010)



DFT + MD / Bonev, Militzer, Galli (2004)



Wave-Packets + MD Erlangen University, Phys.Rev.E (2007)

Theoretical predictions of "dissociative" fluidfluid phase transition in liquid hydrogen



DFT/MD: Scandolo S. *PNAS* **100**, (2003) // Bonev S., Militzer B., Galli G. *PRB* **69** (2004) WPMD : Jakob B. *et al. PRE* (2007) // DFT/MD: Morales M. *et al. PNAS* **107**, (2010)/ DFT/MD: Lorenzen W. *et al. PRB* (2010)

Hypothetical non-congruent phase transitions (*short list*)

Terrestrial applications:

- Uranium- and Plutonium-bearing compounds:
 - UO₂, PuO₂, UC, UN, ... ets.,
- Metallic alloys: (Li-K-Na,...etc.)
- **Oxides**: $(SiO_2...etc.)$
- Hydrides of metals (LiH... etc.)
- Ionic liquids and molten salts:
 alkali halides (NaCl ... etc.), ammonium halides (NH₄Cl ... etc.)...
- "Dusty" and Colloid plasmas: (Coulomb system of macro-ions +Z and micro-ions: +1, -1)



- Plasma and Dissociative Phase Transitions in mixtures: H₂ / He / H₂0 / NH₃ / CH₄ in Giant Planets, Brown Dwarfs and Extra-Solar Planets,
- Phase Transitions in White Dwarfs,
- Phase Transitions in Neutron Stars,
- Phase Transitions in "Strange" Stars (quark-hadron transition ... ets.)



EMMI : Cosmic Matter in the Laboratory

The question is:

What kind of phase transition one can expect in high-*T*_high-*P* complex plasma ?

 $SiO_2 + FeO + Al_2O_3 + CaO + \dots$



Natural and artificial bombarding of lunar surface





Launch – April 24, 2009 Impact velocity ~ 9'000 km/h 🗇 Impact plume ~ 50 km high

What kind of phase transition one can expect in high- T_h igh-Pcomplex plasma? SiO₂ + FeO + Al₂O₃ + CaO $T \sim eV \& P \sim GPa$

The question is open

<u>NB</u> !

Any phase transition in such mixture must be *non-congruent*



Exploration of the Moon Continues!

, 2009 // Impact – 9 October 2009



LCROSS Lunar CRater Observation and Sensing Satellite

What kind of phase transition one can expect in high- T_high-P complex plasma? SiO₂ + FeO + Al₂O₃ + CaO $T \sim eV \& P \sim GPa$

The question is open

<u>NB</u> !

Phase transition in each constituent (SiO₂, FeO, Al₂O₃, CaO...) must be *non-congruent* !

Phase transitions in the mixture must be *non-congruent* moreover !



4 V , 4/66

Impact and fireball hydrodynamics in HIC



Hypothetical non-congruent phase transitions (*short list*)

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Density, g/cm3

Non-Congruence in Cosmic Matter:

- Plasma Phase Transitions in mixture: H₂/ He /H₂0 / NH₃ / CH₄ in Giant Planets, Brown Dwarfs and Extra-Solar Planets,
- Phase Transitions in White Dwarfs,
- Phase Transitions in Neutron Stars,
- Phase Transitions in "Strange" Stars (quark-hadron transition ... ets.)

Non-congruence *of* hypothetical "plasma phase transition" *in* molten salts



а, b, c, d — тройные и критические точки; однородные фазы: TT — твердое тело; Г — газ, ИЖ — ионная жидкость; МЖ — молекулярная жидкость; П — плазма, ПП — плотная плазма. T₁ — температура плавления;



Non-congruence in exotic situations



(di scussi on)

Non-congruence *in* compact stars *and* supernova explosions

Compact stars

White dwarfs, Neutron stars, "Strange" (quark) stars, Hybrid stars





Hypothetical non-congruence in compact stars and supernova explosions





- "Gas-Liquid" phase transitions
 - Quark-Hadron phase transitions

(after D.Blaschke, "Extreme Matter", Elbrus-2010)

(di scussi on)



Hypothetical non-congruence in compact stars and supernova explosions

EMMI



"Gas-liquid" PT in "low-density" nuclear matter



Evident contradiction

Calculated phase transitions are of ordinary VdW type (congruent)

"Gas-liquid" PT in "low-density" nuclear matter (di scussi on)



S. Typel, G. Roepke, D. Blaschke et al. Phys. Rev. C, 81 (2010)

Evident contradiction

Calculated phase transitions are of ordinary VdW type (congruent)

"Gas-liquid" PT in "low-density" nuclear matter (di scussi on)



S. Typel, G. Roepke, D. Blaschke et al. Phys. Rev. C, 81 (2010)

Phase transition in **symmetric** *p*-*n*-*N*(*A*,*Z*) nuclear matter is **congruent**

Aseotropic composition

"Gas-liquid" PT in "low-density" nuclear matter (di scussi on)







Non-congruence in compact stars



(di scussi on)

Quark-hadron phase transition



I.L.I. / Int. Conf. "Critical Point and Onset of Deconfinement", JINR, Dubna, Russia, 2010

Hypothetical quark-hadron phase transition is it CONGRUENT or NON-CONGRUENT ?



Hypothetical phase transitions in ultra-dense matter: are they <u>CONGRUENT</u> or <u>NON-CONGRUENT</u> ?



I.Iosilevskiy: "*Physics of Neutron Stars*", St.-Pb. Russia, 2008 // EMMI-Workshop_Max Born Symposium, Wroclaw, 2009 // <u>arXiv:1005.4192</u>

Hypothetical phase transitions in ultra-dense matter: are they <u>CONGRUENT</u> or <u>NON-CONGRUENT</u> ?



Hypothetical phase transitions in ultra-dense matter: are they <u>CONGRUENT</u> or <u>NON-CONGRUENT</u> ?



Hypothetical phase diagram with Triple or Quadruple Point

R. Pisarski & L. McLerran: EMMI-Wroclaw /2009/, QCD-Bad Honnef /2010/

Hypothetical phase transitions in ultra-dense matter:
are they CONGRUENT or NON-CONGRUENT ?



What is this – **Triple** and **Quadruple** points in **Non-Congruent** phase transition?

I.Iosilevskiy: EMMI-Wroclaw /2009/, QCD-Bad Honnef /2010/

Hypothetical phase transitions in ultra-dense matter

are they <u>CONGRUENT</u> or <u>NON-CONGRUENT</u> ?



Quark-Hadron Phase Diagram

The problem of non-congruence for Quark-Hadron phase transition is relevant to physics of super-colliders!

Iosilevskiy I. / "Critical Point and Onset of Deconfinement", JINR, Dubna, Russia, 2010

Impact and fireball hydrodynamics in HIC



Conclusions and **Perspectives**

- Non-congruent phase transition is general phenomenon

- Non-congruent phase transition is universal phenomenon

- Non-congruent phase transition is interesting phenomenon

- It is **promising** to investigate non-congruent phase transitions **experimentally**. in particular with **intense laser** and **heavy ion** heating

 It is promising to investigate non-congruent phase transitions in direct numerical simulations ("numerical experiment") DFT/MD, PIMC, WP/MD...

 If one takes into account hypothetical non-congruence of phase transitions in astrophysical objects (*planets, compact stars etc.*) he should revise totally the scenario of all phase transformations in these objects



Non-Congruent Phase Transitions in Cosmic Matter and Laboratory

Thank you!



RAS Scientific Programs:

"Physics of Extreme States of Matter" *and* "Physics of Compressed Matter and Interiors of Planets" Extreme Matter Institute - EMMI

Acknowledgements

Support Vladimir Fortov (*Russia*) Claudio Ronchi (*Germany*) Boris Sharkov (*Russia*) Dieter Hoffmann (*Germany*)

RAS Scientific Program: "Physics and Chemistry of Extreme States of Matter"

MIPT Research & Educational Center "High Energy Density Physics"

Extreme Matter Institute - EMMI

Collaboration (INTAS 1995-2002): Victor Gryaznov (*Russia*) Eugene Yakub (*Ukraine*) Alexander Semenov (*Russia*) Vladimir Youngman (="=) Lev Gorokhov (="=) Michael Brykin (="=) Michael Brykin (="=) Michael Zhernokletov (="=) Michael Zhernokletov (="=) Temur Salikhov (*Uzbekistan*)

Gerard J. Hyland (Warwick, UK)

INTAS 93-66 // ISTC 2107, 3755 // CRDF MO-011